

Ferrous Application I

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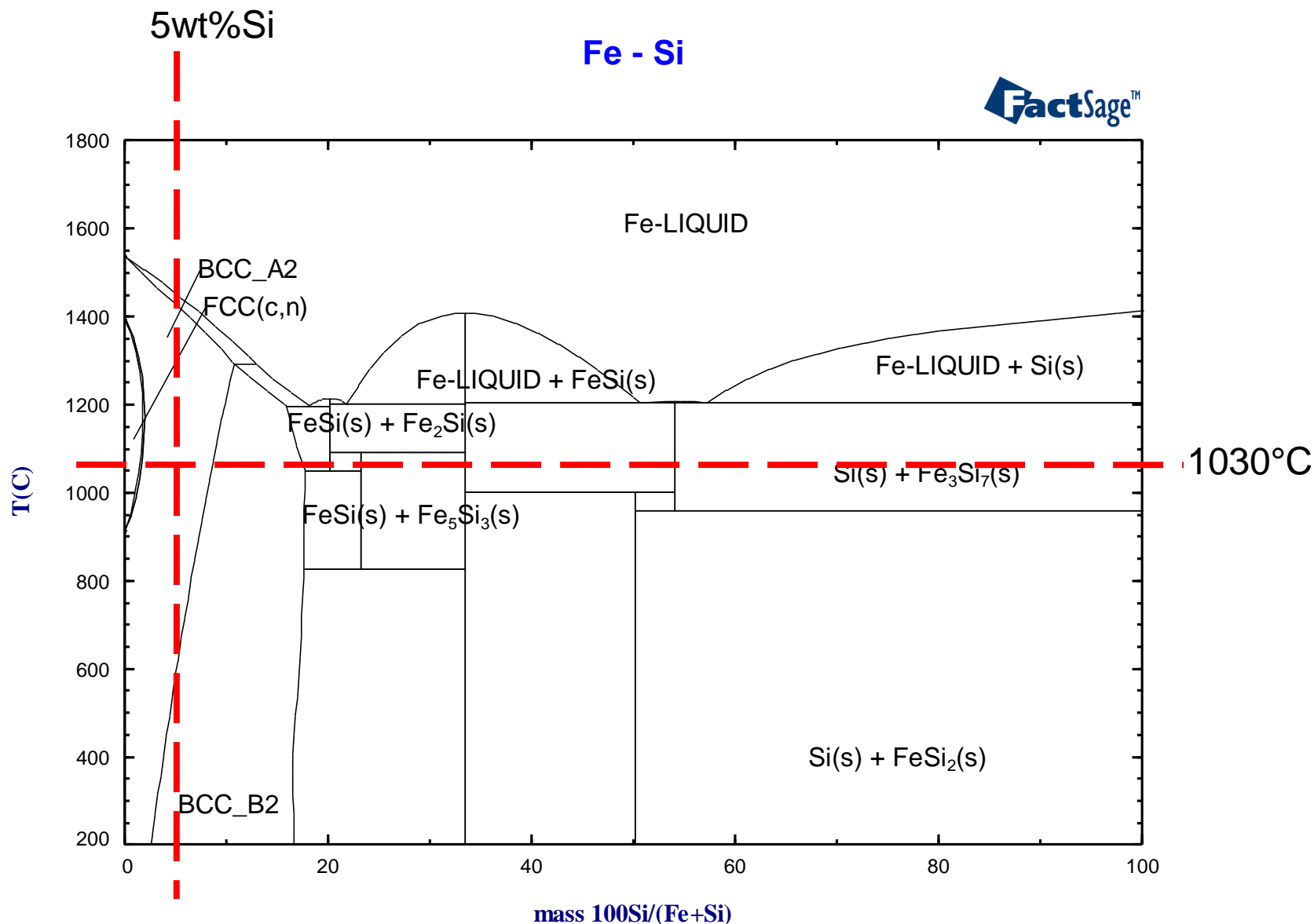
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Simple calculation examples of Equilib module

Fe-Si binary phase diagram - Fe-5wt.% Si at 1030 °C



FactSage™

Reactants Window - Fe-Si at Fe-5wt.% Si

Reactants Window

Equilib - Reactants

File Edit Table Units **Data Search** Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
95	Fe				1	
+ 5	Si				1	

Next >>

FactSage 8.0 Compound: 1/23 databases Solution: 1/23 databases

Data Search

Data Search

Databases - 1/23 compound databases, 1/23 solution databases

FactSage[®] **SGTE**

FactPS FScoep BINS compounds only Private Databases
 FToxid FSlead SGPS solutions only EXAM SGTEa SGTEb
 FTsalt FSstel SGTE no database
 FTmisc FSuopt SGsold
 FTball Other
 FT0xCN ELEM SGnobl
 FTfrtz FTdemo SpMCBN
 FThelp TDmeph
 FTpulp FTnucl TDnucl
 FTlite

Information -

Options - search for product species

Include compounds
 gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits
Organic species CxHy... X(max) =
Minimum solution components: 1 2 cpts

Menu Window - Fe-5wt.% Si at 1030 °C

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(gram) 95 Fe + 5 Si

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids** 14

species: 14

Target: **Pure solids**

Estimate T(C): 1000
Quantity(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10	steps	1030	1	

1 calculation

Equilibrium

- normal
- normal +
- transitions only
- no time limit -

Calc

FactSage 8.0

Solution phases

*	+	Base-Phase	Full Name
I		FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
I		FSstel-BCC2	BCC_B2IBCC_A2
+		FSstel-DIAM	Diamond_A4

Selection of solid phases

Selection - Equilib - no results -

File Edit Show Sort

Selected: 14/14 **SOLID**

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	3	Si(s)	FSstel	diamond_A4	V				
+	4	Si(s2)	FSstel	bcc_A2	V				
+	5	Si(s3)	FSstel	fcc_A1	V				
+	6	Si(s4)	FSstel	cbcc_A12	V				
+	7	Si(s5)	FSstel	cub_A13	V				
+	8	Si(s6)	FSstel	hcp_A3	V				
+	9	Si(s7)	FSstel	hcp_Zn	V				
+	10	Fe(s)	FSstel	BCC_A2	o				
+	11	Fe(s2)	FSstel	FCC_A1	o				
+	12	FeSi(s)	FSstel	FeSi_11_-18262	o				
+	13	FeSi2(s)	FSstel	FeSi2_<FeSi2_L	o				
+	14	Fe2Si(s)	FSstel	Fe2Si	o				
+	15	Fe3Si7(s)	FSstel	Fe3Si7	o				
+	16	Fe5Si3(s)	FSstel	Fe5Si3	o				

permitted selection of X species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

Results Window - Fe-5wt.% Si at 1030 °C

Equilib - Results 1030 C

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

FactSage 8.0

```
(gram) 95 Fe + 5 Si =
100.00 gram BCC_A2#1
(100.00 gram, 1.8792 mol)
+ 0 gram BCC_A2#2
(1030 C, 1 atm, a=1.0000)
( 95.000 wt.% Fe
+ 5.0000 wt.% Si)

System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Fe                      1.7011          95.000           0.90526            0.95000
Si                      0.17803         5.0000           9.4738E-02         5.0000E-02

+ 0 gram BCC_B2#1
+ 0 gram BCC_B2#2
(1030 C, 1 atm, a=1.0000)
( 86.000 wt.% Fe1Fe1Va6
+ 6.7632 wt.% Fe1Si1Va6
+ 6.7632 wt.% Si1Fe1Va6
+ 0.47369 wt.% Si1Si1Va6)

Site fraction of sublattice constituents:
Fe                      0.90526      Stoichiometry = 1
Si                      0.094738
```

<A>		T(C)	P(atm)	Product H(J)
		1030	1	

1 calculation

Calculate >>

Fe-5wt.% Si transition calculations: "Transition"

Equilib - Menu: File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2): (gram) 95 Fe + 5 Si

Products

Compound species: gas ideal real 0; aqueous 0; pure liquids 0; pure solids 14; species: 14

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FSstel-BCC2	BCC_B2BCC_A2
	+	FSstel-DIAM	Diamond_A4

Custom Solutions: 0 fixed activities, 0 ideal solutions

Pseudonyms: apply Edit ...

Volume data: assume molar volumes of solids and liquids = 0; include molar volume data and physical properties data

paraequilibrium & Gmin: edit

Total Species (max 5000): 38
Total Solutions (max 200): 10
Total Phases (max 1500): 24

Transitions - temperature: Number of transitions: All

Legend: I - immiscible 3; J - 3-immiscible 1; +- selected 1; Show all selected; species: 24; solutions: 10

Equilibrium: normal; normal + transitions; transitions only; open; - no time limit - Calculate >>

Final Conditions: <A> T(C) P(atm) Product H(J); 200 1800 200 1; 10 steps; Table; 9+ calculations

Equilib - Results 200 C (page 1/12)

Equilib - Results 200 C (page 1/12): T(C) P(atm) Energy(J) Quantity(g) Vol(litre); 400 C | 590.35 C | 600 C | 800 C | 1000 C | 1200 C | 1400 C | 1439.25 C | 1463.79 C | 1600 C | 1800 C

FactSage 8.0

(gram) 95 Fe + 5 Si =

100.00 gram BCC_B2#1
(100.00 gram, 0.93958 mol)
(200 C, 1 atm, a=1.0000)
(85.153 wt.% FeFe1Va6
+ 14.482 wt.% FeSi1Va6
+ 0.31676 wt.% SiFe1Va6
+ 4.7977E-02 wt.% SiSi1Va6)

Site fraction of sublattice constituents:

Element	Site fraction	Stoichiometry
Fe	0.99507	1
Si	4.9258E-03	

Element	Site fraction	Stoichiometry
Fe	0.81545	1
Si	0.18455	

System component

Component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7011	95.000	0.90526	0.95000
Si	0.17803	5.0000	9.4738E-02	5.0000E-02

+ 0 gram BCC_B2#2

Final Conditions: <A> T(C) P(atm) Product H(J); 200 1800 200 1; 9+ calculations; Calculate >>

Fe-5wt.% Si from 200 °C to 1800 °C every 200 °C

Phase transformation calculations

- “Transition”:
 - select “Transition” for calculation mode.
 - most simple way to calculate all transition of T or X at given range set by user.
for X (composition), set <A> to component in Reactant window.
 - FactSage will show all specific conditions when transitions occur.
- “Precipitation” target:
 - Set “P” option for target phase.
 - FactSage will decrease temperature and find at which temperature another phase starts to form from the target phase. For example, if Liquid is target phase, “P” target will give liquidus temperature.
- “Formation” target:
 - Set “F” option for target phase.
 - FactSage will increase temperature and find at which temperature the target phase begin to form. For example, if Liquid is target phase, “F” target will give solidus temperature.

Fe-5wt.%Si target for liquid phase: "Formation target"

Equilib - Menu: File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2): (gram) 95 Fe + 5 Si

Products

Compound species: gas ideal real 0, aqueous 0, pure liquids 0, pure solids 14, species: 14

Formation Target: FSstel-Liqu, Estimate T(C): 1000, Quantity(g): 0

Final Conditions: T(C) 1439.25, P(atm) 1, Product H(J) 1 calculation

Solution phases:

*	+	Base-Phase	Full Name
	IF	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FSstel-BCC2	BCC_B2 BCC_A2
	+	FSstel-DIAM	Diamond_A4

Legend: I - immiscible 3, J - 3-immiscible 1, F - formation target, + - selected 1

Equilibrium: normal

Equilib - Results 1439.25 C

Output Edit Show Press Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

(gram) 95 Fe + 5 Si =

100.00 gram BCC_A2#1
(100.00 gram, 1.8792 mol)
+ 0 gram BCC_A2#2
(1439.25 C, 1 atm, a=1.0000)
(95.000 wt.% Fe
+ 5.0000 wt.% Si)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7011	95.000	0.90526	0.95000
Si	0.17803	5.0000	9.4738E-02	5.0000E-02

+ 0 gram LIQUID#1
+ 0 gram LIQUID#2
(1439.25 C, 1 atm, a=1.0000)
(93.471 wt.% Fe
+ 6.5286 wt.% Si)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0	0	0.87805	0.93471
Si	0	0	0.12195	6.5286E-02

+ 0 gram BCC_B2#1
+ 0 gram BCC_B2#2
(1439.25 C, 1 atm, a=1.0000)
(86.000 wt.% Fe|Fe|Va6
+ 6.7632 wt.% Fe|Si|Va6
+ 6.7632 wt.% Si|Fe|Va6
+ 0.47369 wt.% Si|Si|Va6)

Site fraction of sublattice constituents:
Fe 0.90526 Stoichiometry = 1
Si 9.4738E-02

Fe 0.90526 Stoichiometry = 1
Si 9.4738E-02

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0	0	0.87805	0.93471
Si	0	0	0.12195	6.5286E-02

Final Conditions: T(C) 1439.25, P(atm) 1, Product H(J) 1 calculation

Calculate >>

F – formation target phase

Fe-5wt.%Si target for liquid phase: "Precipitation target"

Equilib - Menu:

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(gram) 95 Fe + 5 Si

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 14

species: 14

Precipitate Target

FSstel-Liqu

Estimate T(C): 1000

Quantity(g): 0

Final Conditions

<A> T(C) P(atm) Product H(J)

10 steps Table 1 calculation

FactSage 8.0

Solution phases

*	+	Base-Phase	Full Name
		IP	FSstel-Liqu
		J	FSstel-FCC
		I	FSstel-BCC
		I	FSstel-BCC2
		+	FSstel-DIAM

Legend

I - immiscible 3

J - 3-immiscible 1

P - precipitate target

+ - selected 1

Equilibrium

normal

transitions

- no time limit

P – precipitate target phase

Equilib - Results 1463.79 C

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

FactSage 8.0

(gram) 95 Fe + 5 Si =

100.00 gram LIQUID#1
(100.00 gram, 1.8792 mol)

+ 0 (1463.79 C, 1 atm, a=1.0000)
(95.0000 wt.% Fe
+ 5.0000 wt.% Si)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7011	95.000	0.90526	0.95000
Si	0.17803	5.0000	9.4738E-02	5.0000E-02

+ 0 gram BCC_A2#1

+ 0 (1463.79 C, 1 atm, a=1.0000)
(96.242 wt.% Fe
+ 3.7585 wt.% Si)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0	0	0.92794	0.96242
Si	0	0	7.2056E-02	3.7585E-02

+ 0 gram BCC_B2#1

+ 0 (1463.79 C, 1 atm, a=1.0000)
(89.307 wt.% Fe1Fe1Va6
+ 5.2112 wt.% Fe1Si1Va6
+ 5.2112 wt.% Si1Fe1Va6
+ 0.27082 wt.% Si1Si1Va6)

Site fraction of sublattice constituents:

Fe	0.92794	Stoichiometry = 1
Si	7.2056E-02	

Fe	0.92794	Stoichiometry = 1
Si	7.2056E-02	

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7011	95.000	0.90526	0.95000
Si	0.17803	5.0000	9.4738E-02	5.0000E-02

Final Conditions

<A> T(C) P(atm) Product H(J)

1 calculation

Calculate >>

Figure -

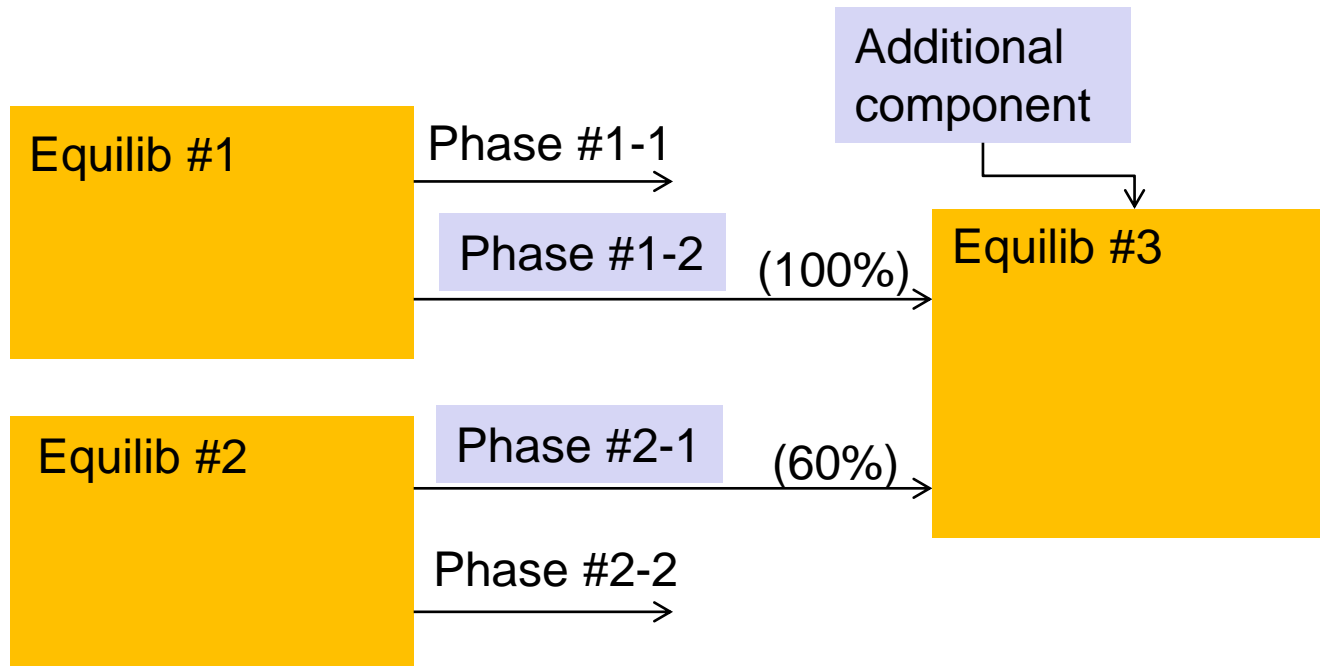
399

Stream

- What is stream and why we need this?

In industrial process, solutions (or mixtures) can be added as reactants. This is called as “stream” (or “mixture”) in FactSage. In order to easily create and add such solutions as input, “stream” can be created from Equilib and it can be added as reactant for next Equilib calculation. Heat and mass of solution(s) are conserved in stream.

* “mixture” can be generated in “Mixture” module in FactSage



Creating new stream : Fe-0.1C-1Mn-1Si at 1600°C

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 4

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
97.9	Fe				1	
+ 0.1	C				1	
+ 1	Mn				1	
+ 1	Si				1	

Initial Condition

Next >>

FactSage 8.0 Compound: 1/26 databases Solution: 1/26 databases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 97.9 Fe + 0.1 C + Mn + Si

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 0

species: 0

Target

- none -

Estimate T(C): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc

Legend

+ - selected 1

Show all selected

species: 4

solutions: 1

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

10 steps Table

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin

Virtual species: 0

Total Species (max 5000): 4

Total Solutions (max 200): 1

Total Phases (max 1500): 1

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

FactSage 8.0

Creating new stream : Fe-0.1C-1Mn-1Si at 1600°C

Save the liquid FeLQ phase as a stream

Equilib - Results 1600 C

Output Edit Show Pages Final Conditions

Save or Print As ... Repeat Save Plot Equilib Results file Stream File Format Fact-XML Fact-Optimal Fact-Function-Builder Refresh ... Swap loops ...

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

FactSage 8.0

Mn + Si =

	Amount/mol	Amount/gram		
	1.7531	97.900	0.96577	0.97901
	1.8202E-02	1.0000	1.0028E-02	1.00001
	3.5606E-02	1.0000	1.9615E-02	
	8.3259E-03	0.10000	4.5868E-03	

Save solutions > ALL solutions Ftmisc-FeLQ Fe-liq

Cut-off limit for phase activities = 1.00E-75

H (J)	G (J)	V (litre)	S (J/K)	Cp (J/K)
1.33719E+05	-2.14956E+05	0.00000E+00	1.86144E+02	8.26499E+01

H (J)	G (J)	S (J/K)
1.33719E+05	-2.14956E+05	1.86144E+02

Fe-liq

Total mass/gram = 100.00

Databases: Ftmisc 8.0

Data Search options: exclude gas ions; organic CxHy.. X(max) = 2; min soln cpts

Final conditions: T(C) = 1600, P(atm) = 1

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

Calculate >>

Save mixture/stream (*.mixt) - enter the file number (1 - 9999) or name

This PC > Local Disk (C:) > Workshop80

Organize New folder

Name	Date modified	Type	Size
ChemSage	12/20/2019 2:05 PM	File folder	
Examples	12/20/2019 1:54 PM	File folder	
F9010	12/23/2019 7:38 PM	File folder	
FACTDATA	12/23/2019 7:37 PM	File folder	
FactHelp	12/20/2019 2:05 PM	File folder	
FactSage-Teach	12/20/2019 2:00 PM	File folder	
Figures	12/20/2019 1:59 PM	File folder	
FSReactor	12/20/2019 2:05 PM	File folder	
Functions	12/20/2019 1:54 PM	File folder	
MACROS	12/20/2019 2:00 PM	File folder	
Myresult	12/23/2019 10:52 AM	File folder	

File name: Feliq.mixt

Save as type: Mixture/stream (*.mixt)

Save Cancel

Save File C:\Workshop80\Feliq.mixt

Saving file Feliq.mixt

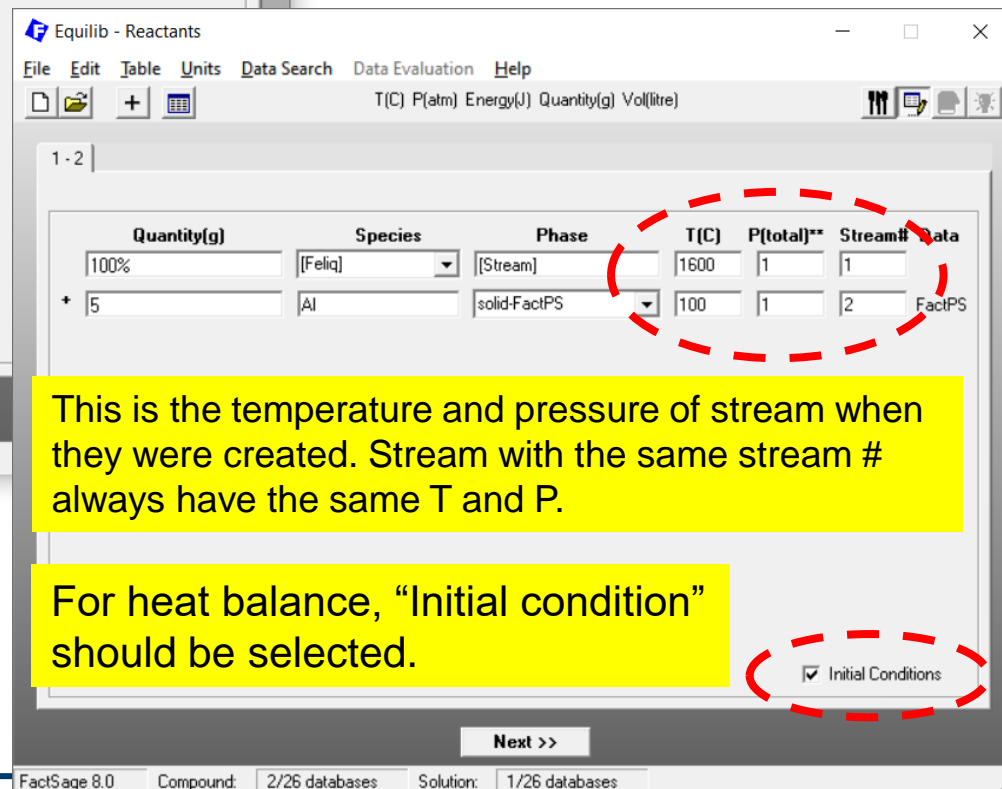
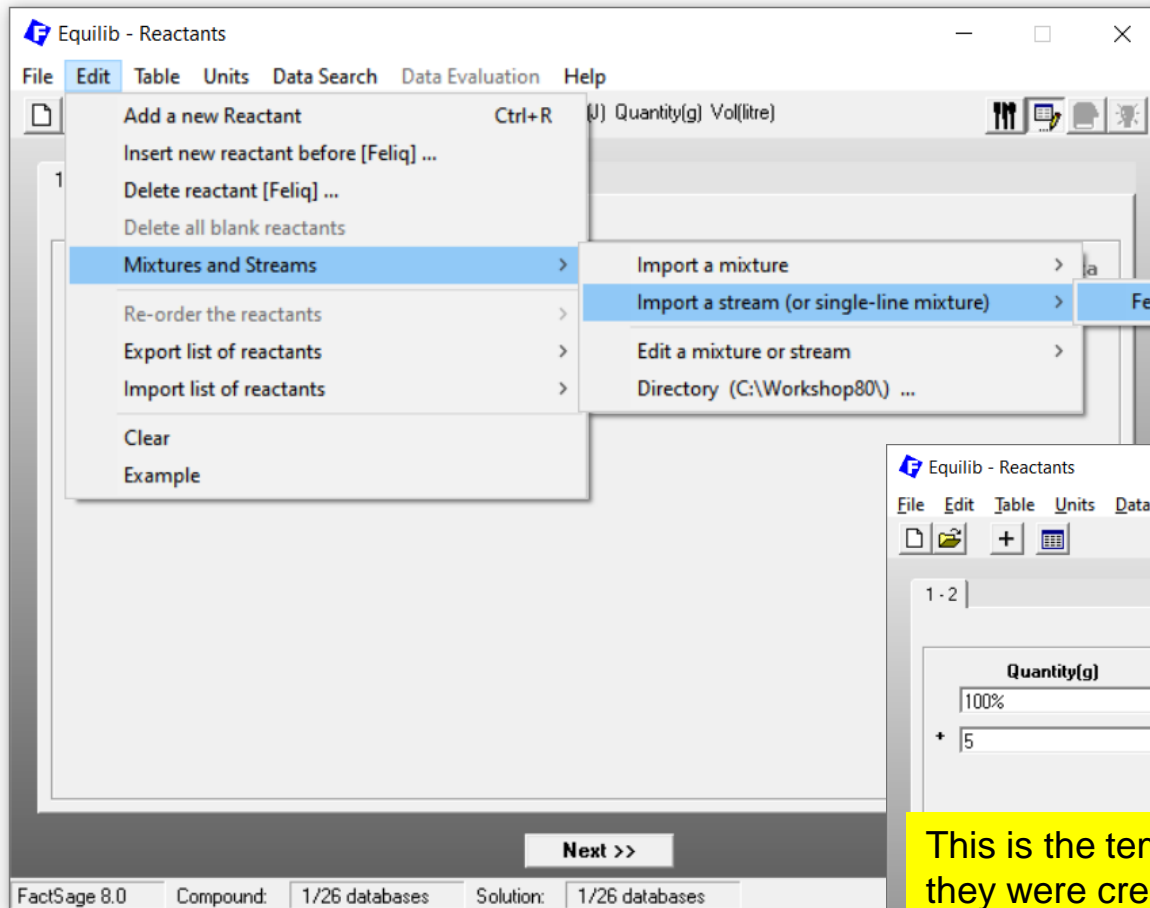
Enter one line of comments

OK Cancel

Ftmisc-FeLQ Fe-liq

www.factsage.com

Import stream : Fe-0.1C-1Mn-1Si at 1600°C



Heat balance: Fe-0.1C-1Mn-1Si(1600°C) + Al (25°C)

Adiabatic calculation :
 $\Delta(H) = 0$
 $\Delta(H) > 0$: heat loss
 $\Delta(H) < 0$: heat gain

The screenshot shows the 'Equilib - Menu: last system' window. The 'Reactants (2)' section contains '(gram) 100% [Feliq] (1600C,#1) + 5 Al (100C,s-FactPS,#2)'. The 'Products' section shows a table of solution phases:

Base-Phase	Full Name
FTmisc-FeLQ	Fe-liq
FTmisc-BCCS	bcc
FTmisc-FCCS	fcc

The 'Final Conditions' table is shown below:

<A>		T(C)	P(atm)	Delta H(J)
			1	0

The 'Equilibrium' section is set to 'normal' with 'no time limit'. A red dashed circle highlights the 'Delta H(J)' column in the 'Final Conditions' table, which contains the value '0'. A '1 calculation' button is visible at the bottom right of the table.

Calculated adiabatic temperature = 1605.5 °C

The screenshot shows the 'Equilib - Results 1605.5 C' window. The 'Output' section displays the following text:

```
(gram) 100% [Feliq] + 5 Al =
(1600, 1, stream, #1) (100, 1, s-FactPS, #2)

105.00 gram Fe-liq
(105.00 gram, 2.0005 mol)
(1605.50 C, 1 atm, a=1.0000)
( 93.238 wt.% Fe
+ 4.7619 wt.% Al
+ 9.5238E-02 wt.% C
+ 0.95238 wt.% Mn
+ 0.95238 wt.% Si)
```

The 'System component' table is shown below:

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7531	97.900	0.87631	0.93238
Mn	1.8202E-02	1.0000	9.0988E-03	9.5238E-03
Si	3.5606E-02	1.0000	1.7798E-02	9.5238E-03
Al	0.18531	5.0000	9.2632E-02	4.7619E-02
C	8.3259E-03	0.10000	4.1619E-03	9.5238E-04

The 'Final Conditions' table is shown at the bottom:

<A>		T(C)	P(atm)	Delta H(J)
			1	0

The 'Calculate >>' button is visible at the bottom right of the 'Final Conditions' table.

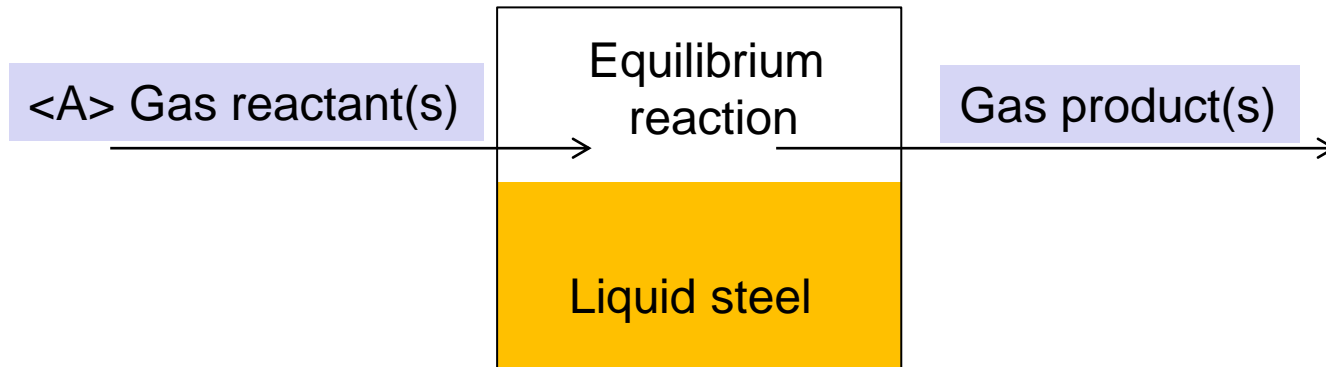
Open calculation

- What is open and why we need this?

In many industrial process, gas are continuously injected and it come out after the reaction with the materials in reactors.

This process can be simulated by “Open” calculation mode.

For activating this <A> for gas species should be assigned in Reactant window.



Repeat this calculation for “Step” times and find the evolution of chemical composition of gas or materials in reactor

No heat balance calculation can be done. Temperature of reactor should be specified by user. Reaction in reactor reaches full equilibrium at each step.

** Open calculation is NOT working with “Stream”*

Open Calculation - off-gas removal

RH – Vacuum degassing process

The screenshot shows the FactSage Equilib software interface. The main window displays the following information:

- Reactants (5):** (gram) 97.9 Fe + 0.1 C + Mn + Si + <A> O2
- Products:** A list of solution phases including FTmisc-FeLQ (Fe-liq), FTmisc-BCCS (bcc), FTmisc-FCCS (fcc), FToxid-SLAGA (A-Slag-liq all oxides + S), FToxid-SLAG? (?-Slag-liq), FToxid-SPINB (B-Spinel), FToxid-MeO_B (B-Monoxide), and FToxid-cPyrA (A-Clinopyroxene).
- Final Conditions:** T(C) = 1600, P(atm) = 0.01, 10 steps.
- Equilibrium:** The 'open' option is selected under the 'Equilibrium' section.

Additional callouts in the image include:

- A yellow box at the top left containing the text: "RH – Vacuum degassing process".
- A yellow box in the middle left containing the text: "Oxygen injection: 10 times of 0.1 gram/each".
- A yellow box at the bottom right containing the text: "Fe-0.1C-1Mn-1Si + O2 at 1600°C and 0.01 atm".

Red boxes highlight the 'Final Conditions' table and the 'Equilibrium' section in the software interface.

<A>		T(C)	P(atm)	Product H(J)
0.1		1600	0.01	
10	steps			10 calculations

Equilibrium options: normal, normal + transitions, transitions only, open

Open Calculation - results

Equilib - Results Step 10 (page 10/10)

Output Edit Show Pages Final Conditions



T(C) P(atm) Energy(J) Quantity(g) Vol(litre)



Step 1 | Step 2 | Step 3 | Step 4 | Step 5 | Step 6 | Step 7 | Step 8 | Step 9 | - Step 10 -

```
+ 4.5715E-23 O3
+ 1.8641E-31 C4
+ 4.1137E-33 Fe(CO)5
+ 2.4932E-35 C5)
```

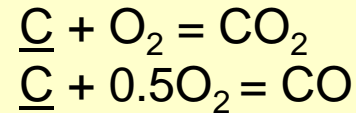
```
+ 98.839 gram Fe-liq
(98.839 gram, 1.7765 mol)
(1600 C, 1.0000E-02 atm, a=1.0000)
( 98.992 wt.% Fe
+ 2.2278E-03 wt.% C
+ 0.65443 wt.% Mn
+ 7.5768E-03 wt.% O
+ 0.34245 wt.% Si
+ 1.5068E-04 wt.% SiO
+ 8.3395E-04 wt.% MnO)
```

System component	Amount/mol	Amount/gram	Mole fraction
Fe	1.7520	97.843	0.98621
Mn	1.1786E-02	0.64747	6.6339E-03
Si	1.2055E-02	0.33856	6.7855E-03
O	4.8307E-04	7.7288E-03	2.7191E-04
C	1.8333E-04	2.2020E-03	1.0320E-04

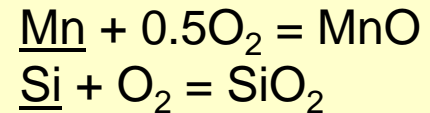
```
+ 1.0279 gram Slag-liq#1
(1.0279 gram, 1.5840E-02 mol)
(1600 C, 1.0000E-02 atm, a=1.0000)
( 52.051 wt.% SiO2
+ 6.6205 wt.% FeO
+ 4.2485E-03 wt.% Fe2O3
+ 41.320 wt.% MnO
+ 4.1169E-03 wt.% Mn2O3)
```

```
Site fraction of sublattice constituents:
Si 0.56215
Fe2+ 5.9798E-02
Fe3+ 3.4529E-05
Mn2+ 0.37798
Mn3+ 3.3844E-05
```

Carbon content decreases due to the reactions:



New slag formed due to Si and Mn oxidation:



Open Calculation - plot of log(wt% liquid steel)

1 Plot

2 Axes

3 Y-axis

4 Y-axis

5 Select

Activity list:

- activity
- mole
- mole fract.
- gram
- weight %
- Alpha
- T(C)
- P(atm)
- Cp(J)
- G(J)
- Vol(litre)
- H(J)
- V(litre)
- S(J)
- page -
- Y
- log10(Y)
- ln(Y)
- exp(Y)
- 1/Y
- phase distribution

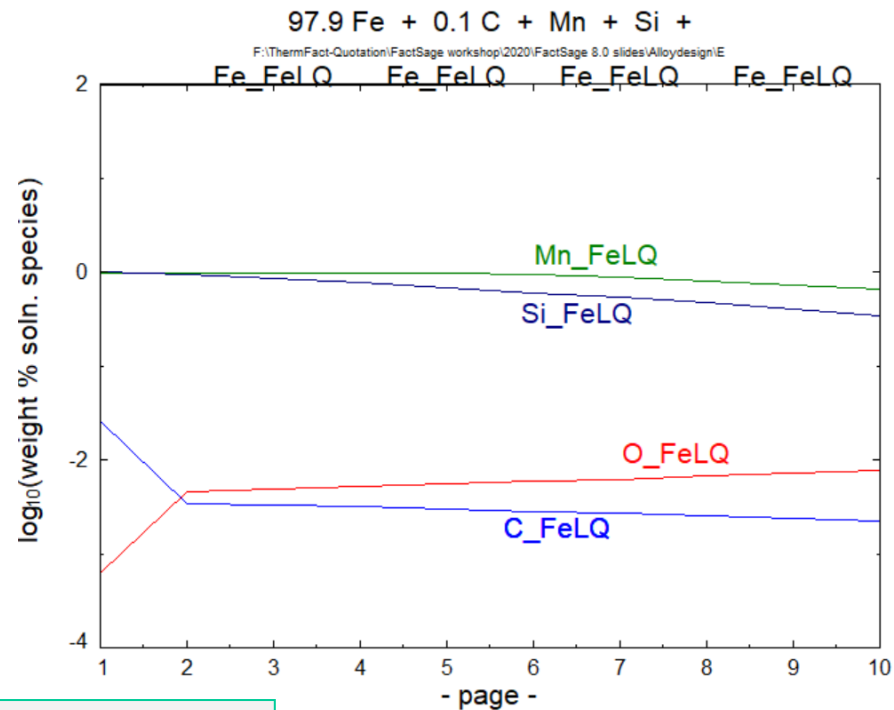
Axes	Variables	Minimum	Maximum
	activity	0	1
	mole	0	1.8087
	mole fract. soln. species	0	1
	gram	0	99.905
Y-axis	weight % soln. species	0	100
	Alpha	0	0
	T(C)	1600	1600
	P(atm)	1.0000E-02	1.0000E-02
	Cp(J/K)	83.645	89.199
	G(J)	-2.3687E+05	-2.1680E+05
	Vol(litre)	0.192237	101.17
	H(J)	1.1237E+05	1.3309E+05
	V(litre)	0.192237	101.17
X-axis	- page -	1	10

Open Calculation - log(wt%) vs page

Plot Species Selection - Equilib Results: log₁₀(weight % soln. species) vs - page -

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
23	FeO	2.1368E-11					
24	Fe(CO)5	4.3734E-38					
FeLQ		Fe-liq					
25	Fe	1.752					
26	C	1.8333E-04					
27	Mn	1.1774E-02					
28	O	3.6801E-05					
29	Si	1.2051E-02					
30	SiO	9.0100E-07					
31	MnO	1.3013E-06					
SLAGA #1		A-Slag-liq all oxid					
32	SiO2	0	8.9046E-03	0.56217	0.996231	1.9409E-02	0.962847
33	FeO	0	9.4721E-04	7.4877E-04	5.9800E-02	2.4521E-03	3.2426E-02
34	Fe2O3	0	2.7347E-07	2.9711E-07	1.7265E-05	2.8137E-11	6.3830E-08
35	MnO	0	5.9873E-03	3.0168E-03	0.393552	6.9465E-03	6.5998E-02
36	Mn2O3	0	2.6805E-07	3.5648E-06	1.6922E-05	3.1535E-11	3.3932E-08
SLAGA #2		A-Slag-liq all oxid					

Do NOT select this.
This is species (modeling) in FeLQ
(for example, SiO and MnO are associate model species)



Plot Species Selection - Equilib Results: log₁₀(weight % soln. species) vs - page -

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
161	Rhod	0	0	0	0	1.0156E-03	0.478955
ELEMENTS							
162	Fe_GAS	1.0183E-07	5.2895E-05	4.1347E-03	4.1745E-03	0	0
163	Mn_GAS	5.3507E-07	3.2056E-04	1.7417E-02	2.5653E-02	0	0
164	Si_GAS	4.7613E-07	1.1396E-04	4.0931E-03	2.7626E-02	0	0
165	O_GAS	1.1894E-05	6.2112E-03	0.485516	0.490629	0	0
166	C_GAS	1.1355E-05	6.1560E-03	0.456984	0.481198	0	0
167	Fe_FeLQ	1.752	0.969235	0.986205	0.986205	0	0
168	Mn_FeLQ	1.1786E-02	1.7882E-02	6.6339E-03	9.9006E-03	0	0
169	Si_FeLQ	1.2055E-02	3.5553E-02	6.7855E-03	1.9657E-02	0	0
170	O_FeLQ	3.9003E-05	4.8307E-04	2.1565E-05	2.7191E-04	0	0
171	C_FeLQ	1.8333E-04	2.1699E-03	1.0320E-04	1.1997E-03	0	0
172	Fe_SLAGA#1	0	9.4776E-04	0	2.3352E-02	0	0
173	Mn_SLAGA#1	0	5.9879E-03	0	0.153587	0	0
174	Si_SLAGA#1	0	8.9046E-03	0	0.219509	0	0
175	O_SLAGA#1	0	2.4745E-02	0	0.609759	0	0

Select these elements in FeLQ
These are what we compare with experimental analysis

When we need to fix activity or partial pressure ?

Only a couple of cases when you need to fix activity or partial pressures are listed below. There could be numerous cases other than these.

- In steelmaking process or other pyrometallurgical process, “Slags” play important roles. Slags can contain oxide components having more than 2 oxidation states (for example, iron oxide, FeO and Fe₂O₃). In some case, FactSage cannot determine how much Fe²⁺ and Fe³⁺ exist in molten slags. The best way to resolve this problem is to fix the oxygen partial pressure of oxygen.
- Any case when you have oxides (solid or liquid state) with more than 2 oxidation states, it is better to fix oxygen partial pressure.
- When you study the solubility of gas species in slag, for example sulfur, it is better to fix the partial pressure of S₂ or SO₂ gas like in experiments.
- *If you equilibrate liquid steel (containing O or S) and slag, this can automatically fixing the oxygen or sulfur partial pressure. So, you don't have to fix the partial pressure of gas species.*
- If you want to saturate the slag with Fe, you can fix the activity of Fe = 1 or enter small amount of Fe in the calculations.
- If you want to calculate iso-activity of SiO₂ (or any other component) composition of slag, you can set activity of SiO₂.

Fixed activity of gas and solid species

Selection - Equilib - no results -

File Edit Show Sort

Selected: 9/11 **GAS** Duplicates selected X denotes species excluded by default

no results -

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	1	O(g)	FactPS	gas					
+a	2	O2(g)	FactPS	gas					
+	3	O3(g)	FactPS	gas					
+	4	Cr(g)	FactPS	gas					
+	5	CrO(g)	FactPS	gas					
+	6	CrO2(g)	FactPS	gas					
+	7	CrO3(g)	FactPS	gas					
+	8	Fe(g)	FactPS	gas					
+	9	FeO(g)	FactPS	gas					
X	10	O2(g)	FSstel	gas					
X	11	FeO(g)	FSstel	gas					

2

Fixed Partial Pressure

3

Enter the value of log10(p)
(or for a range of values enter 'first last step') for
2 O2(g).

OK

Cancel

Press [Cancel] if the partial pressure is no longer fixed.

-25 -15 1

Specify the activity of the selected species or set a range of activities (linear or log scale)

1

permit selection of 'X' species Help Suppress Duplicates Edit priority list

Show Selected Select All Select/Clear... Clear OK

Fixed p_{O_2} in Fe-Cr-O₂

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (3)

[gram] <1-A> Fe + <A> Cr + 0 O2

Products

Compound species

gas ideal real 9

aqueous 0

liquids 0

pure solids 17

custom selection species: 26

Target

Estimate T(C): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
+		FSstel-SIGM	SIGMA
I		FToxid-SLAGA	A-Slag-liq all oxides + S
+		FToxid-SPINA	A-Spinel
+		FToxid-MeO_A	A-Monoxide
+		FToxid-CORU	M2O3(Corundum)

Legend

I - immiscible 3

J - 3-immiscible 1

+ - selected 4

Show all selected species: 52 solutions: 13 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.2		1000	1	
10	steps			11 calculations

Equilibrium

normal normal + transitions

transitions only open

no time limit Calculate >>

Custom Solutions

1 fixed activities

0 ideal solutions

paraequilibrium & Gmin edit

Total Species (max 5000) 78

Total Solutions (max 200) 13

Total Phases (max 1500) 31

FactSage 8.0

Fixed partial pressure of a gas : O₂

Results at $\log(pO_2) = -20$
Small amount of Cr₂O₃ can form on top of the Fe-20%Cr alloy

Equilib - Results a=1.00E-20 (page 6/11)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

a=1.00E-16 | a=1.00E-15 |
a=1.00E-25 | a=1.00E-24 | a=1.00E-23 | a=1.00E-22 | a=1.00E-21 | - a=1.00E-20 - | a=1.00E-19 | a=1.00E-18 | a=1.00E-17 |

FactSage 8.0

(gram) <1-A> Fe + <A> Cr + 0 O2 =
+ 8.5523E-02 O2

0 mol gas_ideal
(1000 C, 1 atm, a=6.4283E-10)
(5.8827E-10 Fe
+ 5.4513E-11 Cr
+ 5.0662E-14 CrO
+ 1.1792E-15 FeO
+ 1.8640E-16 CrO2
+ 1.0721E-17 O
+ 1.0000E-20 O2
+ 3.0962E-22 CrO3
+ 3.5759E-40 O3)

+ 0.81471 gram FCC_Al#1
(0.81471 gram, 1.4608E-02 mol)
+ 0 gram FCC_Al#2
+ 0 gram FCC_Al#3
(1000 C, 1 atm, a=1.0000)
(1.8054 wt.% Cr
+ 98.195 wt.% Fe
+ 1.6814E-10 wt.% O)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.4325E-02	0.80000	0.98064	0.98195
Cr	2.8288E-04	1.4709E-02	1.9364E-02	1.8054E-02
O	8.5621E-14	1.3699E-12	5.8612E-12	1.6814E-12

+ 0.27082 gram M2O3 (Corundum)
(0.27082 gram, 1.7818E-03 mol)
(1000 C, 1 atm, a=1.0000)
(99.999 wt.% Cr2O3
+ 9.0268E-04 wt.% Fe2O3)

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.2		1000	1	

11 calculations
Calculate >>

Fixed partial pressure of a gas : O₂

Fixed pO₂ in MgO-Fe_tO-SiO₂ slag

Selection - Equilib - no results -

File Edit Show Sort

Selected: 13/15 GAS Duplicates selected X denotes species excluded by default

- no results -

+ Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	O(g)	FactPS	gas					
+a 2	O2(g)	FactPS	gas					
+ 3	O3(g)	FactPS	gas					
+ 4	Mg(g)	FactPS	gas					
+ 5	Mg2(g)	FactPS	gas					
+ 6	MgO(g)	FactPS	gas					
+ 7	Si(g)	FactPS	gas					
+ 8	Si2(g)	FactPS	gas					
+ 9	Si3(g)	FactPS	gas					
+ 10	SiO(g)	FactPS	gas					
+ 11	SiO2(g)	FactPS	gas					
+ 12	Fe(g)	FactPS	gas					
+ 13	FeO(g)	FactPS	gas					
X 14	O2(g)	FSstel	gas					
X 15	FeO(g)	FSstel	gas					

Fixed Partial Pressure

Enter the value of log10(p)
(or for a range of values enter 'first last step') for
2 O2(g).

Press [Cancel] if the partial pressure is no longer fixed.

-15 0 1

OK Cancel

permit selection of 'X' species Help Suppress Duplicates Edit priority list :

Show Selected Select All Select/Clear... Clear OK

elp

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

(gram) 30 MgO + 20 FeO + 50 SiO2 + 0 O2

nts (4)

and species

13 ideal 0 real 13

aqueous 0

pure liquids 0

pure solids 0

* - custom selection species: 13

Target - none -

Estimate T(C): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FSstel-HCP	HCP_A3
	I	FSstel-BCC2	BCC_B2 BCC_A2
	+	FSstel-DIAM	Diamond_A4
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel

Legend

I - immiscible 5

J - 3-immiscible 1

+ - selected 7

species: 109

solutions: 20

Show all selected

Custom Solutions

1 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 122

Total Solutions (max 200) 20

Total Phases (max 1500) 21

Equilibrium

normal normal + transitions

transitions only open

- no time limit - Calculate >>

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

10 steps Table 1 calculation

FactSage 8.0

Fixed partial pressure of a gas : O₂

Results at log(pO₂) = -15

Equilib - Results a=1.00E-15 (page 1/16)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

a=1.00E-06 | a=1.00E-05 | a=1.00E-04 | a=0.001 | a=0.01 | a=0.1 | Abort

a=1.00E-15 | a=1.00E-14 | a=1.00E-13 | a=1.00E-12 | a=1.00E-11 | a=1.00E-10 | a=1.00E-09 | a=1.00E-08 | a=1.00E-07

Results at log(pO₂) = -10

Equilib - Results a=1.00E-10 (page 6/16)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

a=1.00E-06 | a=1.00E-05 | a=1.00E-04 | a=0.001 | a=0.01 | a=0.1 | Abort

a=1.00E-15 | a=1.00E-14 | a=1.00E-13 | a=1.00E-12 | a=1.00E-11 | a=1.00E-10 | a=1.00E-09 | a=1.00E-08 | a=1.00E-07

Results at log(pO₂) = -2

Equilib - Results a=0.01 (page 14/16)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

a=1.00E-15 | a=1.00E-14 | a=1.00E-13 | a=1.00E-12 | a=1.00E-11 | a=1.00E-10 | a=1.00E-09 | a=1.00E-08 | a=1.00E-07

a=1.00E-06 | a=1.00E-05 | a=1.00E-04 | a=0.001 | a=0.01 | a=0.1 | Abort

(gram) 30 MgO + 20 FeO + 50 SiO2 + 0 O2 =

- 11.350 O2

0 mol gas_ideal (1600 C, 1 atm, a=1.8478E-02)

(1.7175E-02 SiO
 + 1.2912E-03 Mg
 + 1.0634E-05 Fe
 + 5.3611E-07 Si
 + 1.6624E-08 SiO2
 + 7.6234E-10 Si2
 + 2.9585E-10 Mg2
 + 2.6416E-10 MgO
 + 4.5557E-11 FeO
 + 1.8312E-11 Si3
 + 7.4356E-12 O
 + 1.0000E-15 O2
 + 9.0470E-31 O3)

+ 52.647 gram Slag-liq#1 (52.647 gram, 1.0538 mol) (1600 C, 1 atm, a=1.0000)

(58.686 wt.% SiO2
 + 6.0186E-03 wt.% FeO
 + 4.7199E-07 wt.% Fe2O3
 + 41.308 wt.% MgO)

Site fraction of sublattice constituents:

Si 0.48795
 Fe2+ 4.1850E-05
 Fe3+ 2.9532E-09
 Mg 0.51201

 O 1.0000

System component Amount/mol Amount/gram

Fe 4.4107E-05 2.4631E-03
 Si 0.51422 14.442
 Mg 0.53958 13.114

Final Conditions

<A>		T(C)	P(atm)
		1600	1

(gram) 30 MgO + 20 FeO + 50 SiO2 + 0 O2 =

- 0.88232 O2

0 mol gas_ideal (1600 C, 1 atm, a=1.3265E-04)

(8.2981E-05 Fe
 + 4.5733E-05 SiO
 + 3.8076E-06 Mg
 + 1.1242E-07 FeO
 + 1.3998E-08 SiO2
 + 2.3513E-09 O
 + 2.4633E-10 MgO
 + 1.0000E-10 O2
 + 4.5142E-12 Si
 + 2.5726E-15 Mg2
 + 5.4050E-20 Si2
 + 2.8609E-23 O3
 + 1.0933E-26 Si3)

+ 96.022 gram Slag-liq#1 (96.022 gram, 1.7992 mol)

+ 0 gram Slag-liq#2 (1600 C, 1 atm, a=1.0000)

(52.071 wt.% SiO2
 + 16.646 wt.% FeO
 + 3.9976E-02 wt.% Fe2O3
 + 31.243 wt.% MgO)

Site fraction of sublattice constituents:

Si 0.46245
 Fe2+ 0.12364
 Fe3+ 2.6717E-04
 Mg 0.41365

 O 1.0000

System component Amount/mol Amount/gram Mole frac

Fe 0.22296 12.451 5.0315E
 Si 0.83215 23.371 0.18775

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

+ 3.095 (3.095

(gram) 30 MgO + 20 FeO + 50 SiO2 + 0 O2 =

+ 0.48556 O2

0 mol gas_ideal (1600 C, 1 atm, a=1.0024E-02)

(1.0000E-02 O2
 + 2.3513E-05 O
 + 1.0032E-07 FeO
 + 1.3708E-08 SiO2
 + 7.4049E-09 Fe
 + 4.4786E-09 SiO
 + 3.7686E-10 Mg
 + 2.4380E-10 MgO
 + 2.8609E-11 O3
 + 4.4207E-20 Si
 + 2.5201E-23 Mg2
 + 5.1835E-36 Si2
 + 1.0267E-50 Si3)

+ 100.49 gram Slag-liq#1 (100.49 gram, 1.8245 mol)

+ 0 gram Slag-liq#2 (1600 C, 1 atm, a=1.0000)

(49.758 wt.% SiO2
 + 15.564 wt.% FeO
 + 4.8229 wt.% Fe2O3
 + 29.855 wt.% MgO)

Site fraction of sublattice constituents:

Si 0.44864
 Fe2+ 0.11736
 Fe3+ 3.2723E-02
 Mg 0.40129

 O 1.0000

System component Amount/mol Amount/gram Mole fraction Mass fraction

Fe 0.27838 15.546 6.0884E-02 0.15471
 Si 0.83216 23.372 0.18200 0.23259

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

1 calculation

Calculate >>

The amounts of FeO and Fe₂O₃ change with pO₂

Fixed activity of Fe: Fe saturation

Slag (CaO-MgO-SiO₂) and liquid Fe equilibration at 1600°C

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 50 CaO + 10 MgO + 40 SiO₂ + 100 Fe

Products

Compound species

- gas ideal real 16
- aqueous 0
- pure liquids 0
- pure solids 61
- custom selection species: 77

Solution phases

+	Base-Phase	Full Name
+	FTmisc-FeLQ	Fe-liq
I	FToxid-SLAGA	A-Slag-liq all oxides + S
+	FToxid-SPINA	A-Spinel
I	FToxid-MeO_A	A-Monoxide
I	FToxid-cPyA	A-Clinopyroxene
+	FToxid-oPyA	A-Orthopyroxene
+	FToxid-pPyA	A-Propopyroxene
+	FToxid-LcPy	LowClinopyroxene

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

- assume molar volumes of solids and liquids = 0
- include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 224
Total Solutions (max 200) 18
Total Phases (max 1500) 80

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

10 steps Table 1 calculation

Equilibrium

- normal normal + transitions
- transitions only open

- no time limit - Calculate >>

FactSage 8.0

(C) P(atm) Energy(J) Quantity(g) Vol(litre)

FactSage 8.0

```
(gram) 50 CaO + 10 MgO + 40 SiO2 + 100 Fe =
```

```
0
  mol  gas_ideal
  (1600 C, 1 atm, a=1.8023E-04)
  ( 8.2927E-05 Fe
  + 6.6945E-05 Mg
  + 3.0301E-05 SiO
  + 4.5659E-08 Ca
  + 1.1832E-08 FeO
  + 9.7677E-10 SiO2
  + 4.5613E-10 MgO
  + 2.4764E-10 O
  + 2.8398E-11 Si
  + 6.3811E-12 CaO
  + 1.1093E-12 O2
  + 7.9523E-13 Mg2
  + 2.1390E-18 Si2
  + 1.8415E-18 Ca2
  + 2.7217E-24 Si3
  + 3.3423E-26 O3)
```

```
+ 99.763 gram Fe-liq
(99.763 gram, 1.7881 mol)
(1600 C, 1 atm, a=1.0000)
( 99.911 wt.% Fe
+ 1.1790E-09 wt.% Ca
+ 3.1588E-03 wt.% O
+ 8.4849E-02 wt.% Si
+ 1.8983E-06 wt.% Mg
+ 4.1626E-04 wt.% MgO
+ 6.0038E-05 wt.% CaO
+ 1.4963E-05 wt.% SiO)
```

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7848	99.675	0.99819	0.99911
Ca	1.0691E-06	4.2808E-05	5.9736E-07	4.2910E-07
Si	3.0143E-03	8.4657E-02	1.6858E-03	8.4859E-04
Mg	1.0381E-05	2.5232E-04	5.8058E-06	2.5292E-06
O	2.0868E-04	3.3387E-03	1.1670E-04	3.3466E-05

```
+ 85.980 gram Slag-liq#1
(85.980 gram, 1.5562 mol)
+ 0 gram Slag-liq#2
(1600 C, 1 atm, a=1.0000)
( 40.441 wt.% SiO2
+ 48.135 wt.% CaO
+ 0.44691 wt.% FeO
+ 1.3194E-03 wt.% Fe2O3
+ 10.976 wt.% MgO)
```

Site fraction of sublattice constituents:

Si	0.37186
Ca	0.47424
Fe2+	3.4368E-03
Fe3+	9.1296E-06
Mg	0.15045
O	1.0000

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	5.3627E-03	0.29948	1.4528E-03	3.4831E-03
Ca	0.73803	29.579	0.19994	0.34402
Si	0.57871	16.253	0.15678	0.18904

One way to fix Fe saturation in steelmaking calculations is to add a small amount of Fe as an input component

Fixed partial pressure of a gas : Fe saturation and fixed SO₂

Gas / Slag (CaO-MgO-FeO-SiO₂) / Liquid Fe equilibration

The screenshot displays the FactSage 8.0 software interface for an equilibrium calculation. The main window, "Equilib - Menu", shows the reactants as (gram) 40 CaO + 10 MgO + 20 FeO + 30 SiO₂ + 0 O₂ + 0 S₂ + 100 Fe. The products section is currently empty. The "Final Conditions" are set to T(C) = 1600 and P(atm) = 1. The "Equilibrium" options are set to "normal".

The "Selection - Equilib" window shows a list of 33 species. The "GAS" phase is selected, and the list includes various oxides and metals. The "Fixed Partial Pressure" dialog box is open, prompting the user to enter the partial pressure for SO₂(g). The input field contains the value 0.00001.

Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	O(g)	FactPS	gas					
2	O ₂ (g)	FactPS	gas					
3	O ₃ (g)	FactPS	gas					
4	Mg(g)	FactPS	gas					
5	Mg ₂ (g)	FactPS	gas					
6	MgO(g)	FactPS	gas					
7	Si(g)	FactPS	gas					
8	Si ₂ (g)	FactPS	gas					
9	Si ₃ (g)	FactPS	gas					
10	SiO(g)	FactPS	gas					
11	SiO ₂ (g)	FactPS	gas					
12	Si(g)	FactPS	gas					
13	S ₂ (g)	FactPS	gas					
14	S ₃ (g)	FactPS	gas					
15	S ₄ (g)	FactPS	gas					
16	S ₅ (g)	FactPS	gas					
17	S ₆ (g)	FactPS	gas					
18	S ₇ (g)	FactPS	gas					
19	S ₈ (g)	FactPS	gas					
20	SO(g)	FactPS	gas					
21	SO ₂ (g)	FactPS	gas					
22	SO ₃ (g)	FactPS	gas					
23	SSO(g)	FactPS	gas					
24	MgS(g)	FactPS	gas					
25	SiS(g)	FactPS	gas					
26	SiS ₂ (g)	FactPS	gas					
27	Ca(g)	FactPS	gas					
28	Ca ₂ (g)	FactPS	gas					
29	CaO(g)	FactPS	gas					
30	CaS(g)	FactPS	gas					
31	Fe(g)	FactPS	gas					
32	FeO(g)	FactPS	gas					
33	FeS(g)	FactPS	gas					

Fixed partial pressure of a gas : Fe saturation and SO₂

Equilib - Results 1600 C

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

```

+ 1.2397E-11 CaO
+ 3.2246E-12 SO3
+ 7.9550E-14 S1S2
+ 9.8777E-15 S4
+ 4.4331E-15 Si
+ 1.4755E-15 Mg2
+ 4.0464E-20 S5
+ 5.1041E-21 Ca2
+ 1.6795E-21 O3
+ 7.5700E-24 S6
+ 5.2126E-26 S12
+ 1.0865E-27 S7
+ 1.8958E-32 S8
+ 1.0354E-35 S13)

+ 114.68 gram Slag-liq#1
(114.68 gram, 1.9183 mol)
+ 0 gram Slag-liq#2
(1600 C, 1 atm, a=1.0000)
( 25.695 wt.% SiO2
+ 34.259 wt.% CaO
+ 27.381 wt.% FeO
+ 1.7306 wt.% Fe2O3
+ 8.5644 wt.% MgO
+ 0.71215 wt.% S1S2
+ 0.79592 wt.% CaS
+ 0.60503 wt.% FeS
+ 4.0685E-02 wt.% Fe2S3
+ 0.21631 wt.% MgS)

Site fraction of sublattice constituents:
Si 0.25857
Ca 0.36940
Fe2+ 0.23044
Fe3+ 1.3106E-02
Mg 0.12848
-----|
O 0.98226
S 1.7738E-02

System component Amount/mol Amount/gram Mole fraction Mass fraction
Fe 0.47028 26.263 0.10752 0.22900
Ca 0.71330 28.588 0.16308 0.24927
S 4.3333E-02 1.3895 9.9072E-03 1.2116E-02
Si 0.49930 14.023 0.11415 0.12227
Mg 0.24810 6.0300 5.6722E-02 5.2579E-02
O 2.3996 38.392 0.54862 0.33476

+ 90.811 gram Fe-liq
(90.811 gram, 1.6516 mol)
(1600 C, 1 atm, a=1.0000)
( 98.318 wt.% Fe
+ 6.1398E-11 wt.% Ca
+ 0.18224 wt.% O
+ 1.4988 wt.% S
+ 1.0853E-05 wt.% Si
+ 8.1225E-08 wt.% Mg
+ 6.6831E-04 wt.% MgO
+ 1.1781E-04 wt.% CaO
+ 8.7060E-08 wt.% SiO)

System component Amount/mol Amount/gram Mole fraction Mass fraction
Fe 1.5988 89.283 0.96802 0.98318
Ca 1.9078E-06 7.6462E-05 1.1551E-06 8.4200E-07

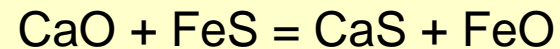
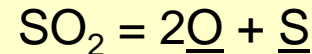
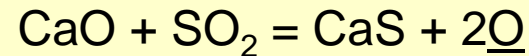
```

Gas (SO₂, S₂, O₂, etc.)

Slag (CaO, MgO, FeO, ...
CaS, MgS, FeS, etc.)

Fe-Lq (O, S, etc.)

Equilibration reactions include:



.....

Composition target: target S content in liquid steel

Composition Target: slag / liquid steel equilibrium

“ How to calculate optimum amount of CaSi to reduce S in liquid steel to a targeted composition”

The screenshot displays the FactSage 8.0 interface. The main window is titled "Equilib - Reactants" and shows a table of reactants with columns for Quantity(g), Species, Phase, and T(C). The table contains the following entries:

Quantity(g)	Species	Phase	T(C)
98.437	Fe		
+	Mn		
+	0,5	Si	
+	0,05	Al	
+	0.003	O	
+	0.01	S	
+	4	CaO	
+	4	Al2O3	
+	2	SiO2	
+	<A>	CaSi	

The "Data Search" dialog box is open, showing a list of databases and options for searching for product species. The "Options - search for product species" section includes:

- Default
- Include compounds:
 - gaseous ions (plasmas)
 - aqueous species
 - limited data compounds (25C)
- Limits:
 - Organic species CxHy... X(max) = 2
 - Minimum solution components: 1 (selected) or 2 cpts

The status bar at the bottom indicates "FactSage 8.0 Compound: 2/26 databases Solution: 2/26 databases".

Composition target: target S content in liquid steel

Selecting target element (species)

Composition Target

Solution MI53-FeLQ

Variable

- species composition
- log10 (species composition)
- element composition
- log10 (element composition)
- species activity
- log10(species activity)
- none (removes targets) -

Species

Code numbers (259-270)
Fe, Al, Ca, ...

259 Fe

Element 2

Elements: O Al Si S Ca Mn Fe

Element: S

Values 3

Enter a single value - or enter a range of values 'first last step'

Element S mass fraction: 0.00002 (0.002%)

Buttons: Cancel, Help, OK

Equilib - Menu

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants [10]

[gram] 98.437 Fe + Mn + 0.5 Si + 0.05 Al + 0.003 O + 0.01 S + 4 CaO + 4 Al2O3 + 2 SiO2 + <A> CaS

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 113
- * - custom selection species: 113

Solution phases

*	+	Base-Phase	Full Name
	C	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS	FeS-liq
		FTmisc-MAT2C	
		FTmisc-PYRRC	
		FTmisc-BCCS	
		FTmisc-FCCS	
		FTmisc-MS-c	

Legend

- ! - immiscible 7
- C - composition target
- element: S
- + - selected 15

Final conditions 4

		T(C)	P(atm)
10 steps		1600	1

Buttons: Cancel, Help, OK

FactSage 8.0

Add CaSi (<A>) to reduce [%S] in Fe-LIQUID to 0.002%.

Composition target: target S content in liquid steel

Amount of CaSi = 0.9674 gram to obtain [%S] = 0.002%

Equilib - Results 1600 C, A=0.9674

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

FactSage 8.0

```
(gram) 98.437 Fe + Mn + 0.5 Si + 0.05 Al +
(gram) 0.003 O + 0.01 S + 4 CaO + 4 Al2O3 +
(gram) 2 SiO2 + <A> CaSi =

100.56 gram Fe-liq
(100.56 gram, 1.8213 mol)
(1600 C, 1 atm, a=1.0000)
( 97.886 wt.% Fe
+ 2.3701E-02 wt.% Al
+ 1.6798E-07 wt.% Ca
+ 0.97619 wt.% Mn
+ 1.5200E-04 wt.% O
+ 2.0000E-03 wt.% S
+ 1.1113 wt.% Si
+ 3.1527E-04 wt.% CaO
+ 2.4610E-04 wt.% AlO
+ 1.1611E-05 wt.% SiO
+ 2.3505E-05 wt.% MnO
+ 2.2014E-05 wt.% Al2O)
```

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7626	98.435	0.96780	0.97886
Mn	1.7869E-02	0.98168	9.8111E-03	9.7621E-03
Ca	5.6572E-06	3.2675E-04	3.1065E-06	2.3549E-06
S	6.2723E-05	2.0112E-03	3.4439E-05	2.0000E-05
Si	3.9790E-02	1.1173	2.1847E-02	1.1113E-02
Al	8.8973E-04	2.4006E-02	4.8852E-04	2.3873E-04
O	2.1879E-05	3.5005E-04	1.2013E-05	3.4810E-06

```
+ 10.407 gram Slag-liq#1
(10.407 gram, 0.15109 mol)
+ 0 gram Slag-liq#2
(1600 C, 1 atm, a=1.0000)
( 38.870 wt.% Al2O3
+ 14.703 wt.% SiO2
```

Table calculations: multi-calculation using EXCEL sheet

- For example, calculations for liquidus temperatures for many slag compositions
- One by one in Equilib using Precipitation target for liquid slag
- Or using **Table** calculation

Perform one calculation to make sure that your calculation is working

The screenshot displays the FactSage 8.0 Equilib interface. The main window shows the following details:

- Reactants (4):** (gram) 45 CaO + 10 MgO + 15 Al2O3 + 30 SiO2
- Products:** A list of solution phases including FToxid-SLAGA (A-Slag-liq all oxides + S), FToxid-SPINA (A-Spinel), FToxid-MeO_A (A-Monoxide), FToxid-cPyrA (A-Clinopyroxene), FToxid-oPyrA (A-Orthopyroxene), FToxid-pPyrA (A-Protopyroxene), FToxid-LcPy (LowClinopyroxene), and FToxid-WOLLA (A-Wollastonite).
- Precipitate Target:** FToxid-SLAGA, Estimate T(C): 1000, Quantity(g): 0.
- Final Conditions:** T(C) 1000, P(atm) 1, Product H(J) 1, 10 steps, 1 calculation.

The results window, titled "Equilib - Results 1518.7 C", shows the following output:

```
(gram) 45 CaO + 10 MgO + 15 Al2O3 + 30 SiO2 =  
  
100.00 gram Slag-liq#1  
(100.00 gram, 1.6970 mol)  
+ 0  
(1518.70 C, 1 atm, a=1.0000)  
( 15.000 wt.% Al2O3  
+ 30.000 wt.% SiO2  
+ 45.000 wt.% CaO  
+ 10.000 wt.% MgO)  
  
Site fraction of sublattice constituents:  
Al 0.15955  
Si 0.27075  
Ca 0.43515  
Mg 0.13454  
O 1.0000  
  
System component Amount/mol Amount/gram Mole fraction Mass fractio  
Ca 0.80246 32.161 0.18513 0.32161  
Si 0.45930 14.023 0.11519 0.14023  
Al 0.29423 7.9388 6.7879E-02 7.9388E-02  
Mg 0.24811 6.0304 5.7240E-02 6.0304E-02  
O 2.4905 39.847 0.57456 0.39847  
  
+ 0  
gram a-(Ca,Sr)2SiO4  
(1518.70 C, 1 atm, a=1.0000)  
( 4.9750 wt.% Mg2SiO4  
+ 95.025 wt.% Ca2SiO4)  
  
System component Amount/mol Amount/gram Mole fraction Mass fractio  
Ca 0 0 0.26850 0.44222  
Si 0 0 0.14286 0.16488
```

Table calculations: multi-calculation using EXCEL sheet

Equilib - Reactants

File Edit **Table** Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 4

Activation of Table

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
45	CaO					
+ 10	MgO					
+ 15	Al2O3					
+ 30	SiO2					

Next >>

FactSage 8.0 Compound: 1/26 databases Solution: 1/26 databases

Equilib - Reactants

File Edit **Table** Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 4

Reaction Table - 1 rows, 4 reactants

Row	T(C)	P(atm)	CaO(gram)	MgO(gram)	Al2O3(gram)	
1	1000	1	45	10	15	30

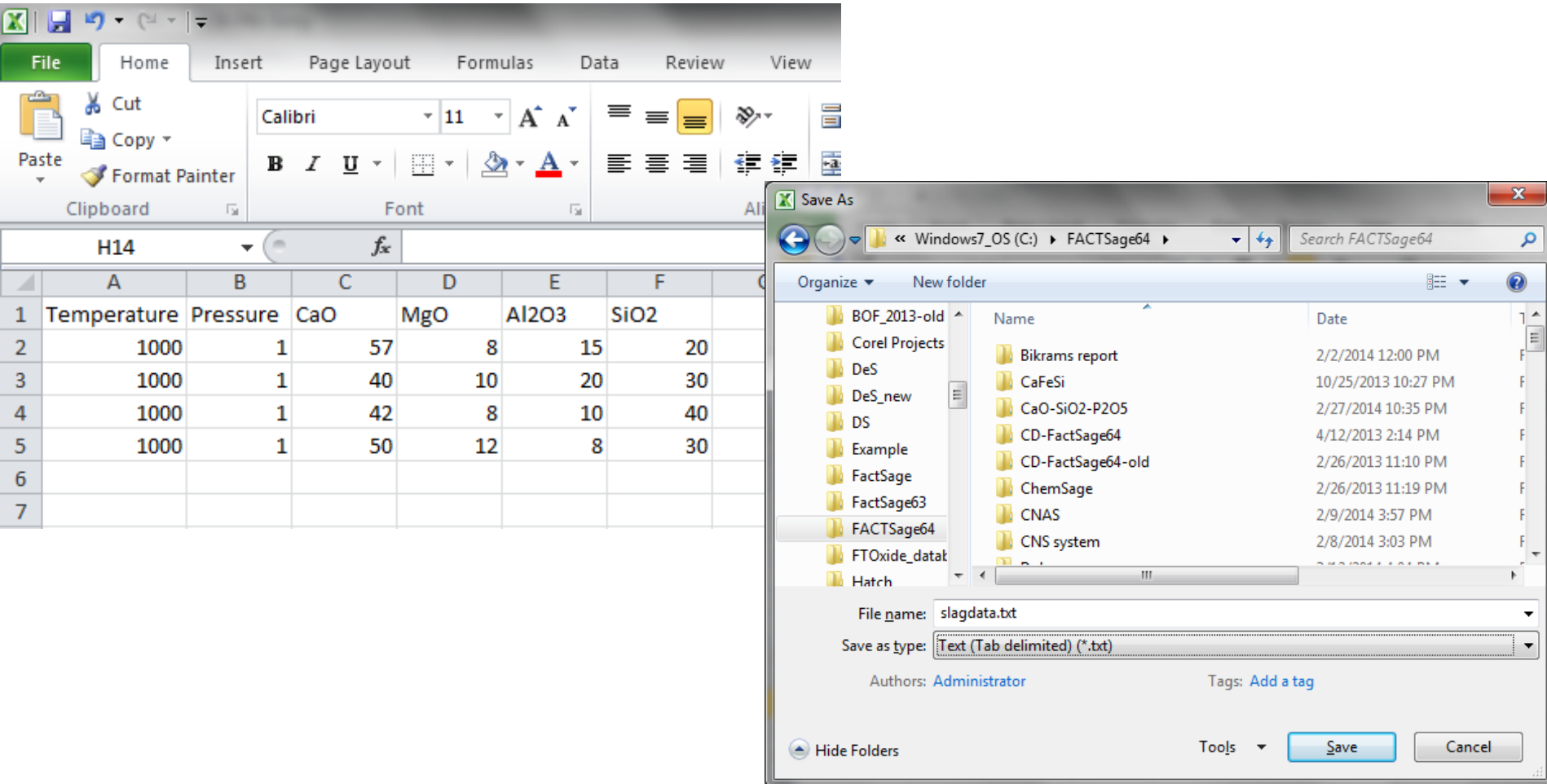
**Check the order of inputs
This order is very important !!**

Next >>

FactSage 8.0 Compound: 1/26 databases Solution: 1/26 databases

Table calculations: multi-calculation using EXCEL sheet

Prepare data in excel spread sheet (input order is the same as the input displayed in FactSage table mode; see previous slide) and then save it as “txt” file



The image shows a screenshot of Microsoft Excel with a data table and a 'Save As' dialog box open. The data table is as follows:

	A	B	C	D	E	F
1	Temperature	Pressure	CaO	MgO	Al2O3	SiO2
2	1000	1	57	8	15	20
3	1000	1	40	10	20	30
4	1000	1	42	8	10	40
5	1000	1	50	12	8	30
6						
7						

The 'Save As' dialog box is open, showing the file name 'slagdata.txt' and the save as type 'Text (Tab delimited) (*.txt)'. The dialog box is located in the 'FACTSage64' folder on the C: drive.

Table calculations: multi-calculation using EXCEL sheet

Import table from text file

The screenshot shows the 'Equilib - Reactants' window with the 'Table' menu open. The 'Import Table' option is highlighted, and a sub-menu is visible with three options: 'from tabular file that includes headers ...', 'from simple text file without headers ...', and 'from clipboard without headers ...'. The background table shows the following data:

Quantity(g)	Vol(litre)
8	15
10	20
8	10
12	8

The screenshot shows the 'Equilib - Reactants' window with the 'Reaction Table' displayed. The table has 4 rows and 4 reactants. The data is as follows:

Row	T(C)	P(atm)	CaO(gram)	MgO(gram)	Al2O3(gram)	Quantity(g)
1	1000	1	57	8	15	20
2	1000	1	40	10	20	30
3	1000	1	42	8	10	40
4	1000	1	50	12	8	30

Table calculations: multi-calculation using EXCEL sheet

The image displays two overlapping windows from the FactSage 8.0 software. The foreground window is titled 'Equilib - Reactants' and has the 'Table' menu open. The menu options include: Reactants Table (Ctrl+T), Help..., Add New Row 2, Add Many New Rows 2..., Insert New Row 1 (Ctrl+I), Duplicate Row 1 (Ctrl+Y), Many Duplicates of Row 1..., Delete Row 1, Delete Rows 1 to..., Clear Table, Export Table, Import Table, Sort Table (first click on any column), Select variable in column 1, Select variable in column 2, and Save and Close Table. The background window is titled 'Equilib - Menu: last system' and shows the reaction: $\text{CaO} + \text{MgO} + \text{Al}_2\text{O}_3 + \text{SiO}_2$. It lists products such as A-Slag-liq all oxides + S, A-Spinel, A-Monoxide, A-Clinopyroxene, A-Orthopyroxene, A-Propyroxene, LowClinopyroxene, and A-Wollastonite. The 'Final Conditions' section shows 10 steps and 4 calculations. The 'Equilibrium' section is set to 'normal'.

Close table input mode
→ Now in the calculation, activate "Table"

Table calculations: multi-calculation using EXCEL sheet

Equilib - Results -1- (page 1/4)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

-1- -2- -3- -4-

FactSage 8.0

(gram) 57 CaO + 8 MgO + 15 Al₂O₃ + 20 SiO₂

100.00 gram Slag-liq#1
(100.00 gram, 1.6949 mol)

+ 0 gram Slag-liq#2
(1784.26 C, 1 atm, a=1.0000)

(15.000 wt.% Al₂O₃
+ 20.000 wt.% SiO₂
+ 57.000 wt.% CaO
+ 8.0000 wt.% MgO)

Site fraction of sublatt

Al 0.15973
Si 0.18071
Ca 0.55181
Mg 0.10776

O 1.0000

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Ca	1.0165	40.737	0.24410	0.40737
Si	0.33287	9.3487	7.9938E-02	9.3487E-02
Al	0.29423	7.9388	7.0659E-02	7.9388E-02
Mg	0.19849	4.8243	4.7667E-02	4.8243E-02
O	2.3220	37.151	0.55763	0.37151

+ 0 gram Monoxide#1
(1784.26 C, 1 atm, a=1.0000)

(1.2670 wt.% CaO
1.0200 wt.% MgO

If you do "calculation", four calculations are done:
Each tab shows the results of each input
→ You can save the results in excel format

J option for FCC phase: Fe steel containing (Ti,Nb)(C,N) ppts

Fe-0.039C-0.01N-0.068Nb-0.018Ti: three possible FCC phases

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (5)

(gram) 99.875 Fe + 0.018 Ti + 0.068 Nb + 0.039 C + 0.01 N

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 18

species: 18

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	-	FSstel-Liq	LIQUID
J		FSstel-FCC	FCC_A1
	-	FSstel-BCC	BCC_A2
I		FSstel-HCP	HCP_A3
+		FSstel-CEME	CEMENTITE
I		FSstel-Me4N	Me4N
I		FSstel-BCC2	BCC_B2 BCC_A2
+		FSstel-M5C2	M5C2

Legend

I - immiscible 7

J - 3-immiscible 1

+ - selected 4

species: 143

solutions: 21

Show all selected

Select

Database: FSstel database

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 161

Total Solutions (max 200) 21

Total Phases (max 1500) 39

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		600 1000 10	1	

10 steps Table 41 calculations

Equilibrium

normal normal + transitions

transitions only open

- no time limit - Calculate >>

FactSage 8.0

J option assume two possible miscibility gap in a solution

J option for FCC phase: Fe steel containing (Ti,Nb)(C,N) ppts

Austenite, Ti and Nb carbo-nitrides are all FCC. In the FSStel database, all these fcc phases are modeled as a single FCC_A1 solution with three possible miscibility gaps.

Equilib - Results 900 C (page 34/44)

Output Edit Show Pages Final Conditions



T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

930 C | 940 C | 950 C | 960 C | 970 C | 980 C | 990 C | 1000 C |
 830 C | 840 C | 850 C | 860 C | 870 C | 880 C | 890 C | 895.31 C | -900 C- | 910 C | 920 C |

99.901 gram FCC_A1#1) **Austenite phase**

```
(99.901 gram, 1.7882 mol)
(900 C, 1 atm, a=1.0000)
( 99.798 wt.% Fe
+ 6.0158E-03 wt.% Nb
+ 2.3491E-06 wt.% Ti
+ 0.18941 wt.% FeC
+ 1.0611E-05 wt.% NbC
+ 4.5898E-09 wt.% TiC
+ 7.0138E-02 gram FCC_A1#2
(7.0138E-02 gram, 8.8433E-04 mol)
(900 C, 1 atm, a=1.0000)
( 1.0260E-03 wt.% Fe
+ 6.5424 wt.% Nb
+ 0.16044 wt.% Ti
+ 1.0799E-02 wt.% FeC
+ 64.000 wt.% NbC
+ 1.7385 wt.% TiC
+ 4.5688E-03 wt.% FeN
+ 26.804 wt.% NbN
+ 0.73833 wt.% TiN)

Site fraction of sublattice com
Fe 2.4898
Nb 0.9543
Ti 4.5424
-----
Va 7.5621
C 0.6551
N 0.2693
```

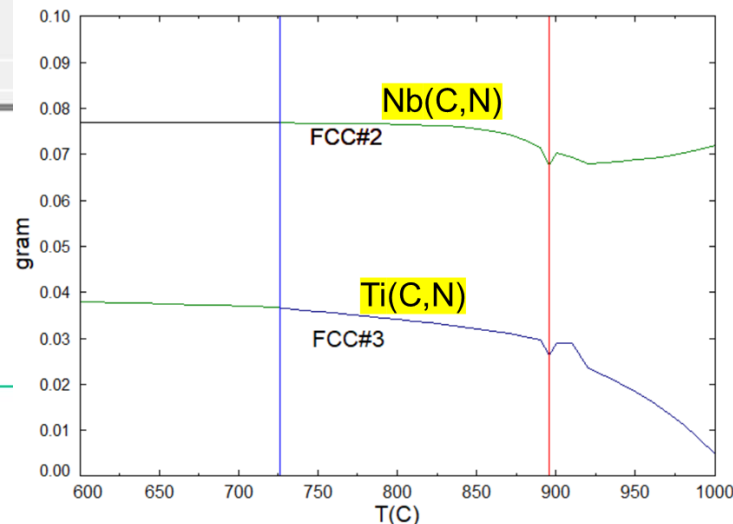
Nb(C,N) ppt.

Ti(C,N) ppt.

```
+ 2.8907E-02 gram FCC_A1#3
(2.8907E-02 gram, 4.4612E-04 mol)
(900 C, 1 atm, a=1.0000)
( 1.0067E-02 wt.% Fe
+ 2.7001E-03 wt.% Nb
+ 3.4144E-02 wt.% Ti
+ 0.46550 wt.% FeC
+ 0.11604 wt.% NbC
+ 1.6255 wt.% TiC
+ 20.570 wt.% FeN
+ 5.0759 wt.% NbN
+ 72.101 wt.% TiN)
```

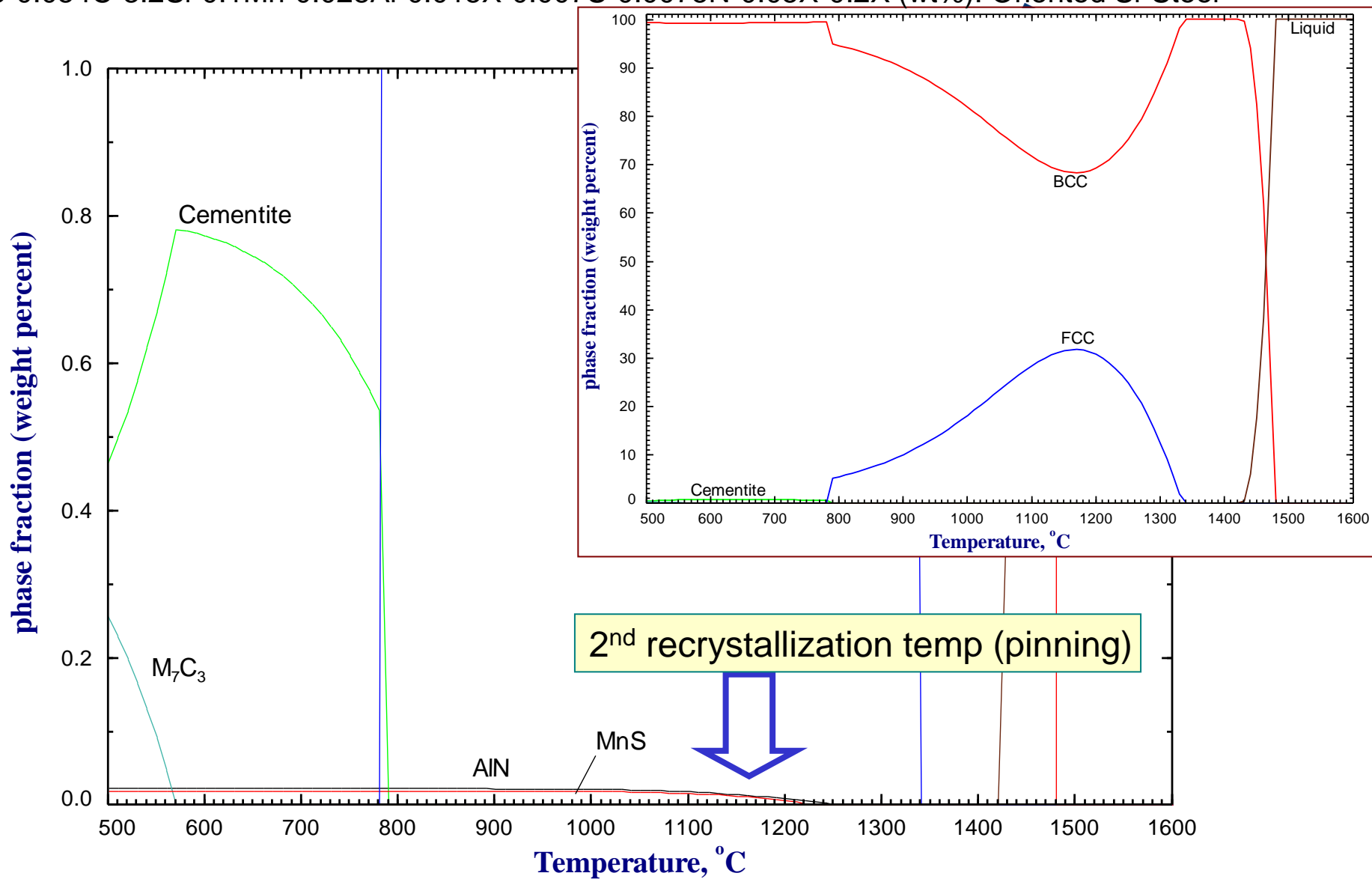
99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C + 0.01N

C:\FactSage73\Equi0.res 13Jan20



Precipitation of AlN and MnS in a commercial Si-steel

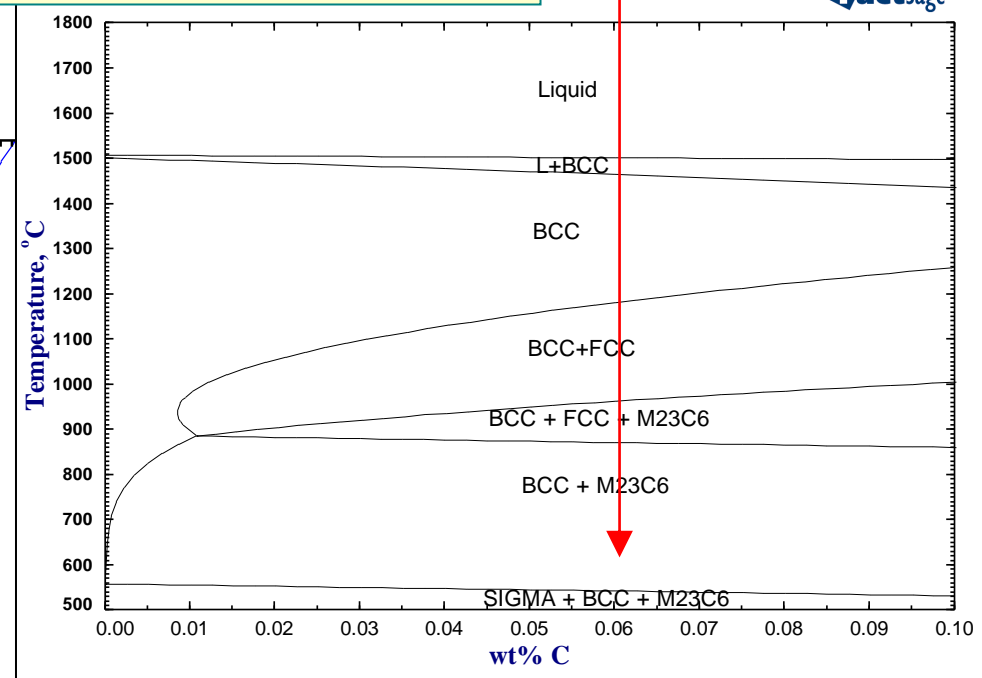
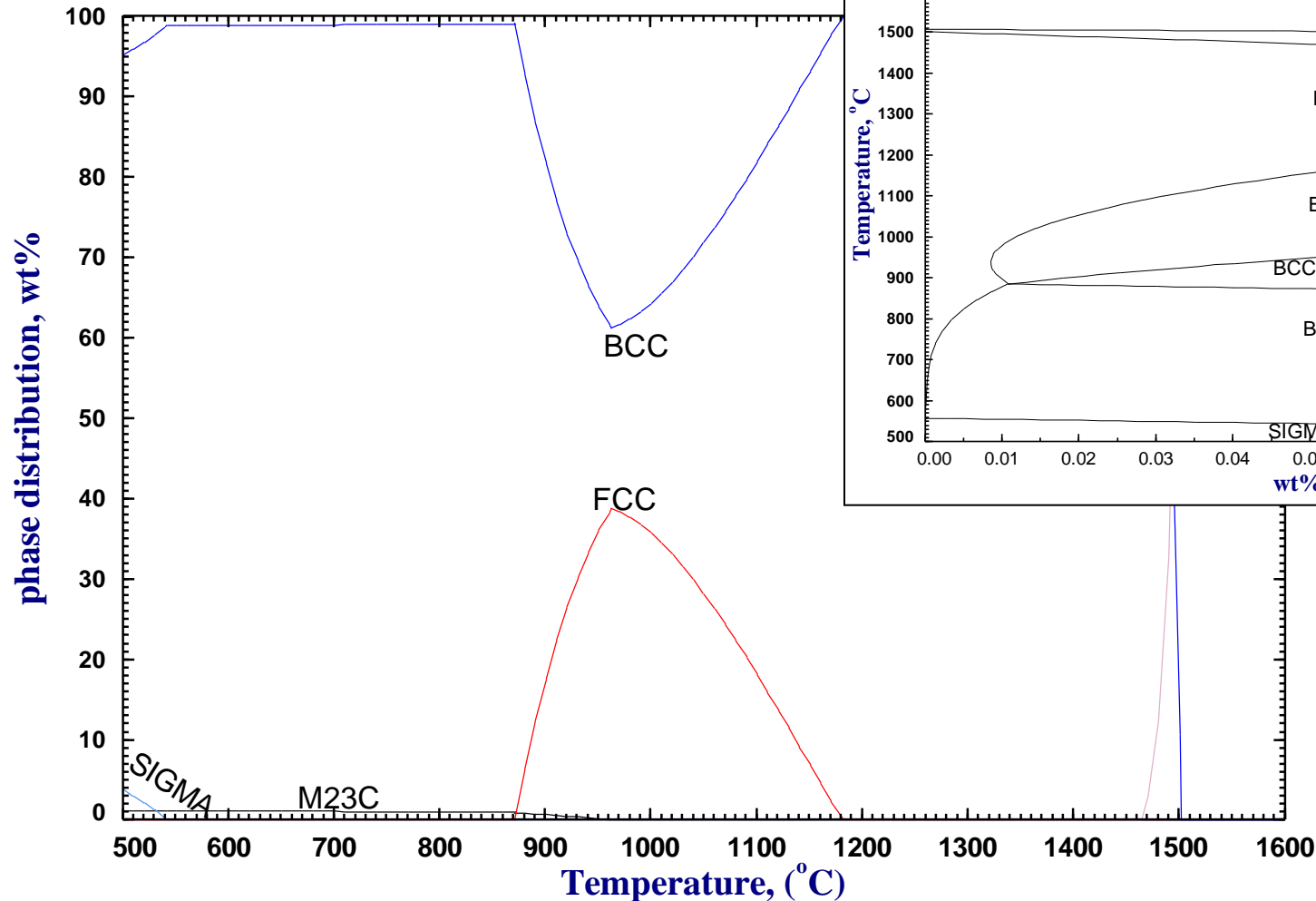
Fe-0.054C-3.2Si-0.1Mn-0.028Al-0.015X-0.007S-0.0075N-0.05X-0.2X (wt%): Oriented Si-Steel



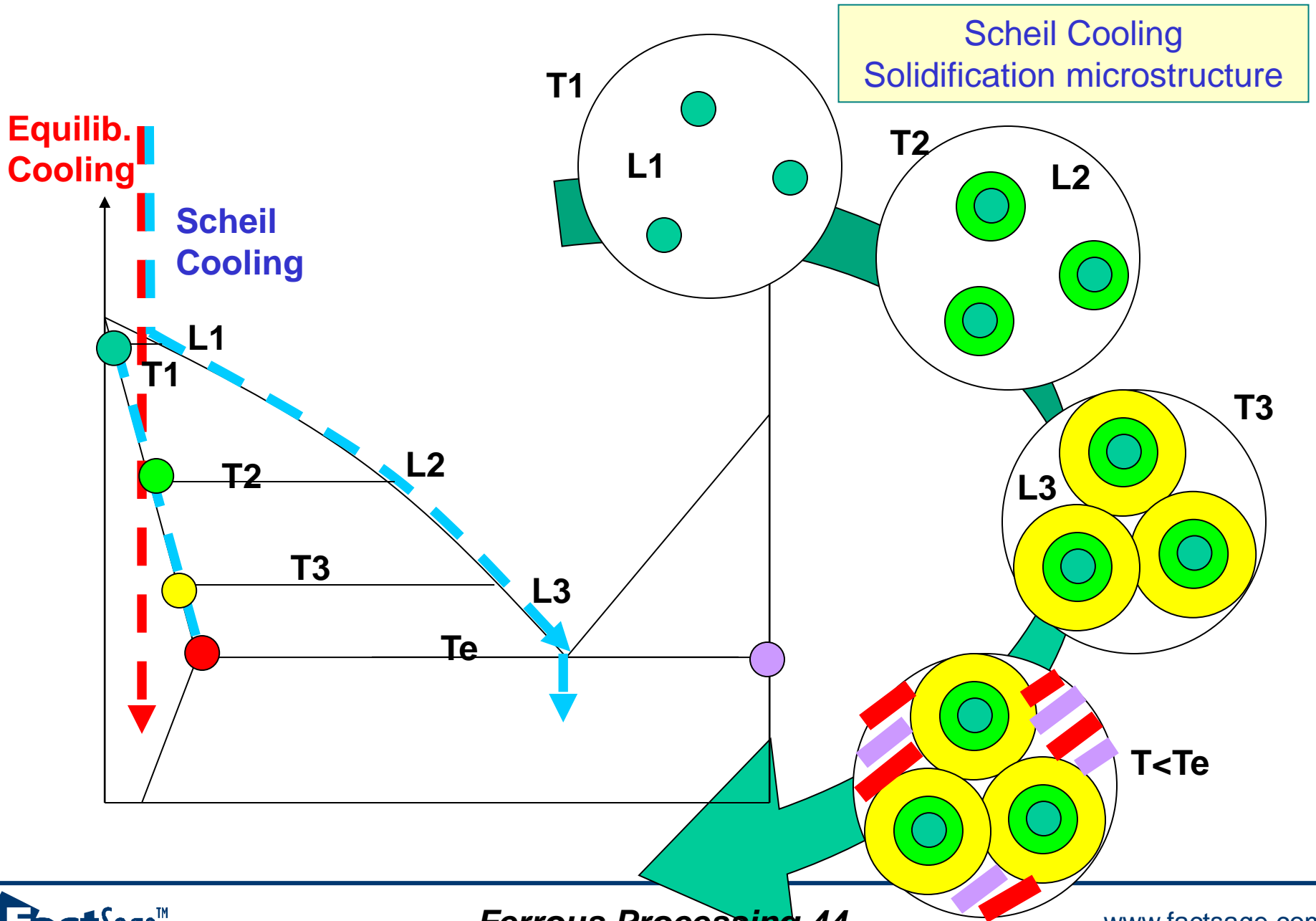
Phase diagram / Phase fraction of 430 Stainless Steel

Fe-16.2Cr-0.06C-0.3Si-0.4Mn-0.3Ni-0.015X(wt%): STS430

FactSage™



Equilibrium cooling and Scheil cooling



Equilibrium solidification of slag

Equilibrium cooling of the CaO-SiO₂-Al₂O₃-MgO slag

Equilib - Reactants

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
40	CaO					
+ 10	MgO					
+ 20	Al2O3					
+ 30	SiO2					

Equilib - Menu: last system

Reactants (4): (gram) 40 CaO + 10 MgO + 20 Al2O3 + 30 SiO2

Products

Compound species: gas ideal real 0; aqueous 0; pure liquids 0; pure solids 50; species: 50

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	I	FToxid-MeO_A	A-Monoxide
	I	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,

Legend: I - immiscible 5; +- selected 9

Final Conditions: T(C) 1600 1000 20; P(atm) 1; Product H(J) [blank]

Equilibrium: normal; normal + transitions; transitions only; open

Calculate >>

Equilibrium solidification of slag: plot amount vs. temperature

1 Plot Results ...

2 Axes

3 Axes: gram vs T(C)

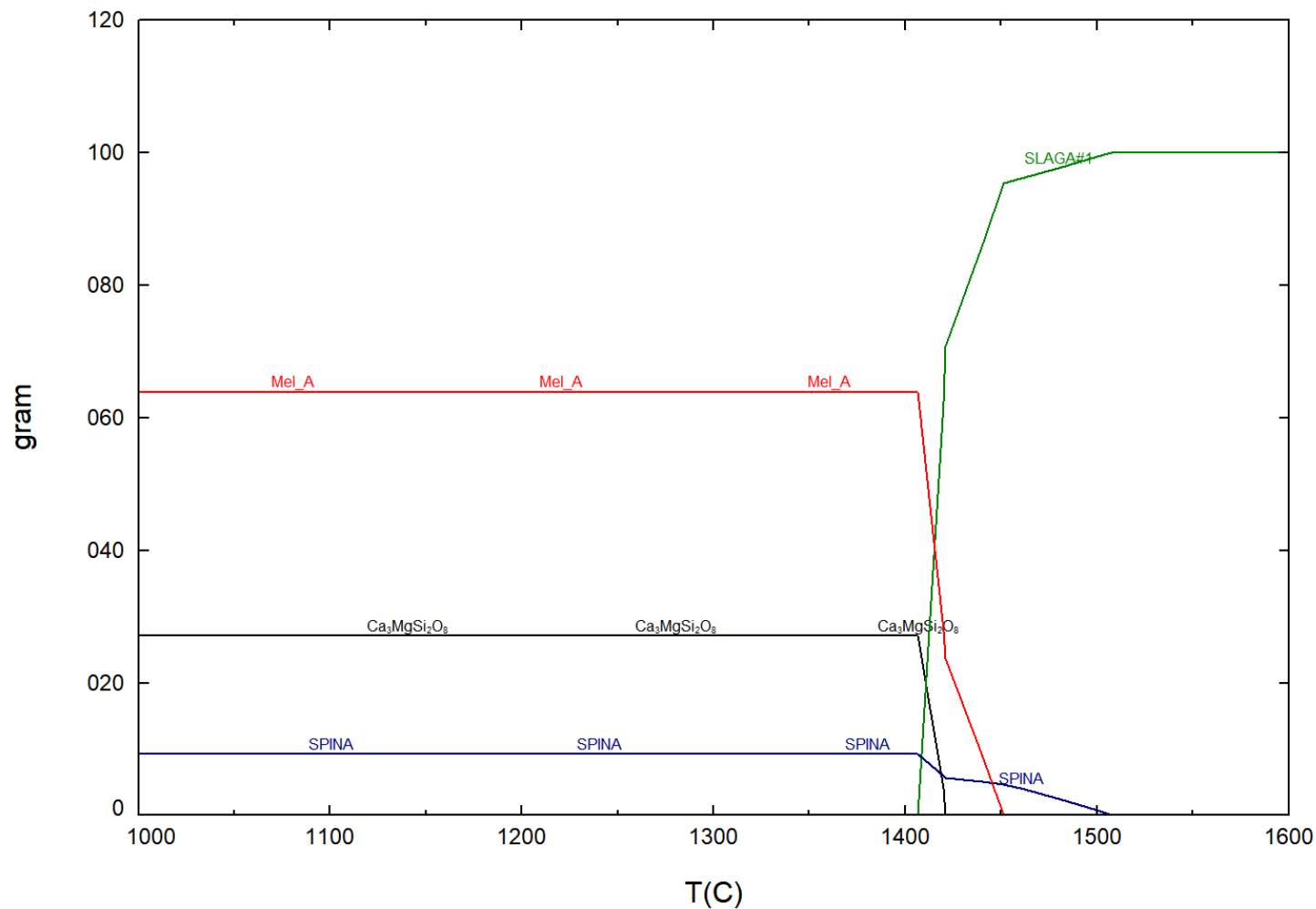
4 4 selected

5 Plot Species Selection - Equilib Results: gram vs T(C)

#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	Activity (max)
126	Ca2MgSi2O7	0	0	0	0	5.7525E-02	0.327122
127	Ca3MgSi2O8	0	27.022	0	0	0.222262	1
128	CaAl2SiO6	0	0	0	0	2.1748E-02	4.9048E-02
129	CaAl2Si2O8	0	0	0	0	2.2597E-08	1.8767E-06
130	CaAl2Si2O8	0	0	0	0	2.2130E-03	1.1561E-02
131	Ca2Al2SiO7	0	0	0	0	0.329637	0.768118
132	Ca3Al2Si3O12	0	0	0	0	3.3125E-05	5.5875E-03
SOLUTIONS							
133	GAS	0	0	0	0	1.8875E-08	1.8875E-08
134	SLAGA#1	0	100	0	0	0.532183	1
135	SLAGA#2	0	0	0	0	0.532183	1
136	SPINA	0	9.1562	0	0	0.545887	1
137	MeO_A#1	0	0	0	0	0.315606	0.595042
138	MeO_A#2	0	0	0	0	2.1860E-02	0.595042
139	cPyxA#1	0	0	0	0	2.5981E-02	9.1098E-02
140	cPyxA#2	0	0	0	0	2.5981E-02	9.1098E-02
141	oPyxA	0	0	0	0	2.7147E-02	6.8979E-02
142	pPyxA	0	0	0	0	2.6509E-02	7.1064E-02

Equilibrium solidification of slag: plot amount vs. temperature

40 CaO + 10 MgO + 20 Al₂O₃ + 30 SiO₂



Equilibrium solidification is completed at ~ 1410°C

Scheil cooling solidification of slag

Scheil cooling of the $\text{CaO-SiO}_2\text{-Al}_2\text{O}_3\text{-MgO}$ slag

Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FToxid-SLAGA

equilibrium cooling

Scheil-Gulliver cooling

normal equilibrium calculation

With Scheil-Gulliver cooling you have the option to apply back diffusion. In the Menu Window select 'apply back diffusion' and click 'edit' to specify the diffusing elements.

Help OK

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 40 CaO + 10 MgO + 20 Al2O3 + 30 SiO2

Solution FToxid-SLAGA

- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from >
- solution properties
- + - single phase
- l - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- C - composition target
- L - cooling calculation

Solution phases

*	+	Base-Phase	Full Name
	IL	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	l	FToxid-MeO_A	A-Monoxide
	l	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,

Legend

l - immiscible 5

L - Scheil cooling

+ - selected 9

Show all selected

species: 82

solutions: 19

Select

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

apply back diffusion edit

Virtual species: 12

Total Species (max 5000) 132

Total Solutions (max 200) 19

Total Phases (max 1500) 69

Equilibrium

normal normal + transitions

transitions only open

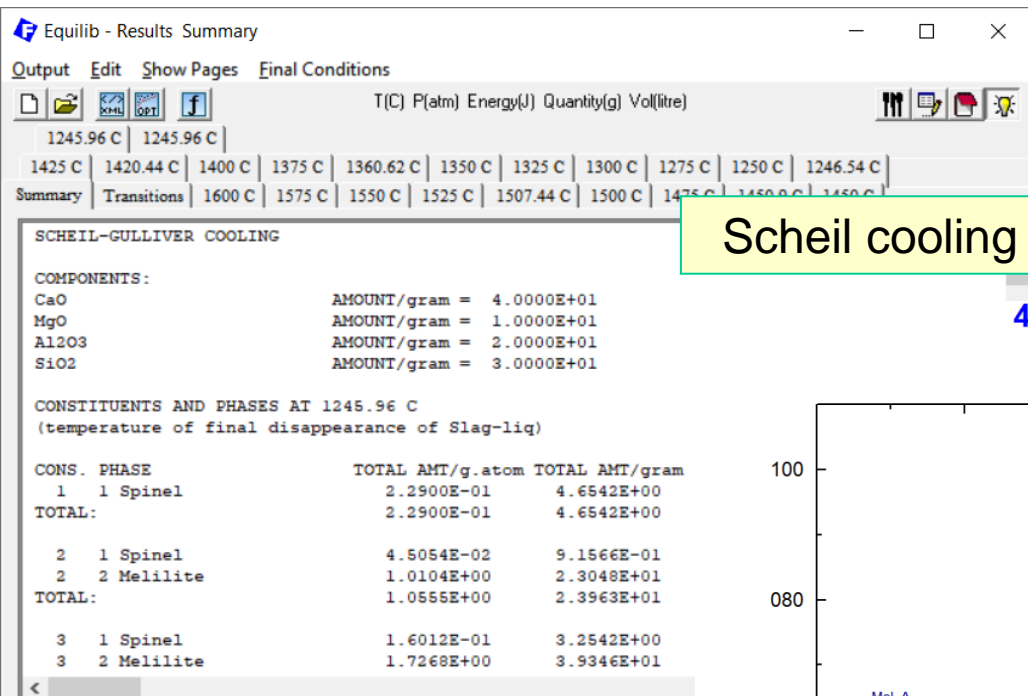
- no time limit - Calculate >>

T(C) P(atm) Product H(J)

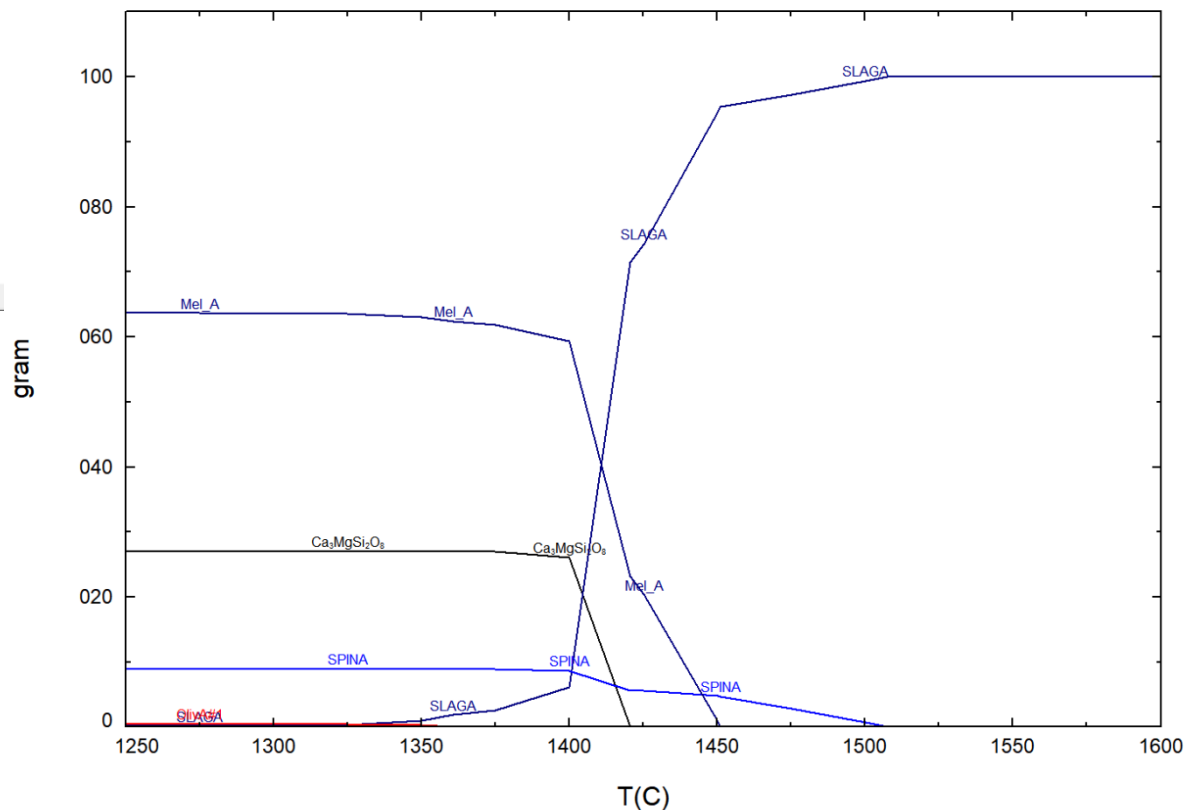
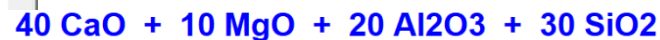
1600 1000 1

Scheil cooling temperature setup: (initial_T final_T)

Equilibrium solidification of slag: plot amount vs. temperature



Scheil cooling solidification is completed at ~ 1320°C



Solidification of mould flux

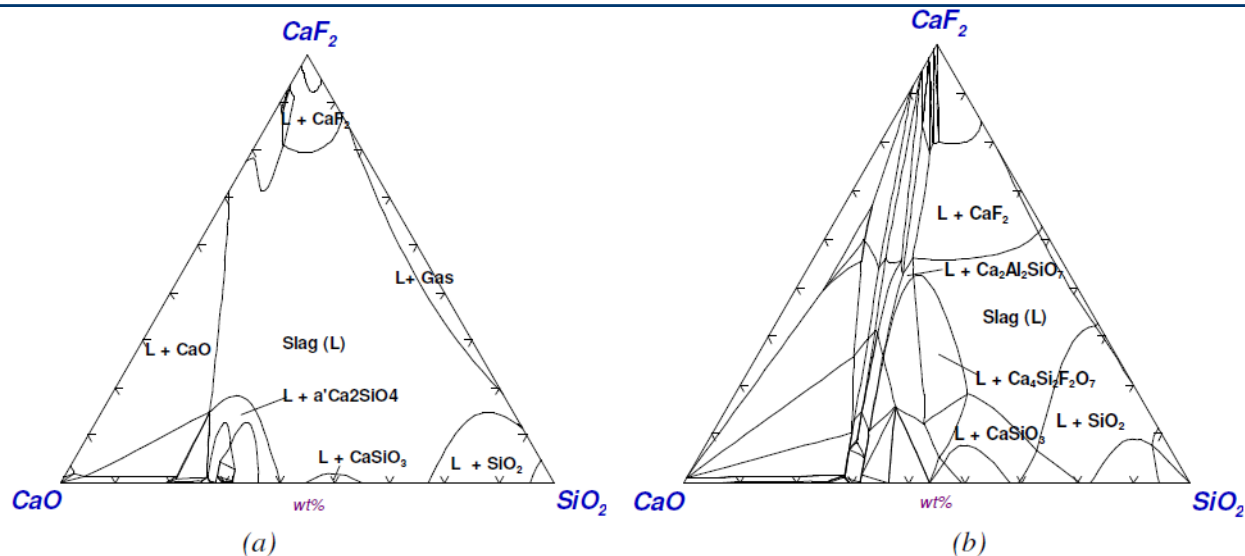


Figure 6. Calculated isothermal phase diagrams for the CaO-SiO₂-CaF₂-10 wt. % Al₂O₃ system at 1 bar [54]. (a) 1400 °C and (b) 1200 °C.

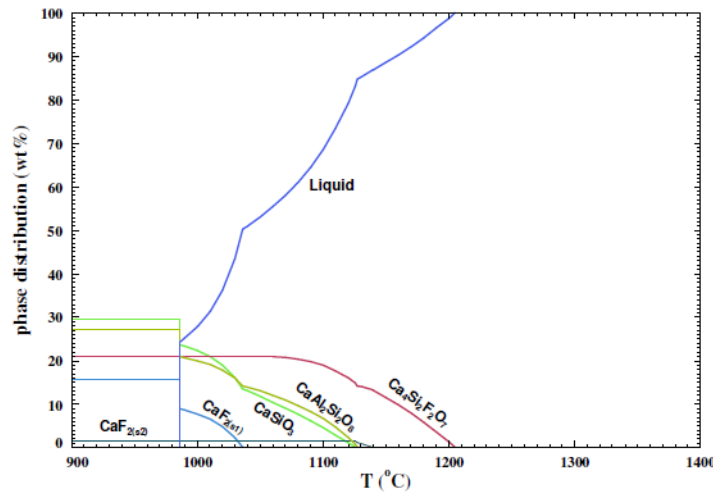


Figure 7. Solidification simulation of the 30CaO-10Al₂O₃-40SiO₂-20CaF₂ (in wt. %) mould flux using the Scheil cooling calculation [16].

Equilibrium solidification of steel: TWIP steel

Equilibrium cooling of Fe-20Mn-1C-1Al TWIP steel

Equilib - Menu: File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 78 Fe + 20 Mn + C + Al

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 33

species: 33

Target

- none -

Estimate ALPHA: 0.5

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FSstel-HCP	HCP_A3
	+	FSstel-CEME	CEMENTITE
	+	FSstel-M23C	M23C6
	+	FSstel-M7C3	M7C3
	+	FSstel-CBCC	CBCC_A12

Legend

- I - immiscible 6
- J - 3-immiscible 1
- + - selected 10

Show all selected

species: 132

solutions: 25

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin

Virtual species: 12

Total Species (max 5000) 165

Total Solutions (max 200) 25

Total Phases (max 1500) 58

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10	steps	1400 1000 10	1	

Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

FactSage 8.0

Equilibrium solidification of steel: TWIP steel

Equilib - Results 1400 C (page 1/81)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1270 C | 1260 C | 1250 C | 1240 C | 1230 C | 1220 C | 1210 C | 1200 C | 1190 C | 1180 C | 1170 C | 1160 C |
 1400 C | 1390 C | 1380 C | 1370 C | 1360 C | 1350 C | 1340 C | 1330 C | 1320 C | 1310 C | 1300 C | 1290 C | 1280 C |

FactSage 8.0

(gram) 78 Fe + 20 Mn + C + Al =

```

100.00 gram LIQUID#1
(100.00 gram, 1.8811 mol)
+ 0 gram LIQUID#2
(1400 C, 1 atm, a=1.0000)
( 1.0000 wt.% Al
+ 1.0000 wt.% C
+ 78.0000 wt.% Fe
+ 20.0000 wt.% Mn)

System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Fe                     1.3967         78.0000          0.74251            0.78000
Mn                     0.36405        20.0000          0.19353            0.20000
Al                     3.7062E-02     1.0000          1.9703E-02         1.0000E-02
C                      8.3259E-02     1.0000          4.4261E-02         1.0000E-02

+ 0 gram FCC_Al#1
+ 0 gram FCC_Al#2
+ 0 gram FCC_Al#3
(1400 C, 1 atm, a=0.98774)
( 1.0004 wt.% Al
+ 82.322 wt.% Fe
+ 14.976 wt.% Mn
+ 2.0551E-02 wt.% AlC
+ 1.4220 wt.% FeC
+ 0.25944 wt.% MnC)

+ 0 gram BCC_A2#1
+ 0 gram BCC_A2#2
(1400 C, 1 atm, a=0.97742)
( 4.8208E-03 wt.% AlC3
+ 1.2805 wt.% Al
+ 0.22282 wt.% FeC3
+ 84.018 wt.% Fe
+ 3.8533E-02 wt.% MnC3
+ 14.436 wt.% Mn)

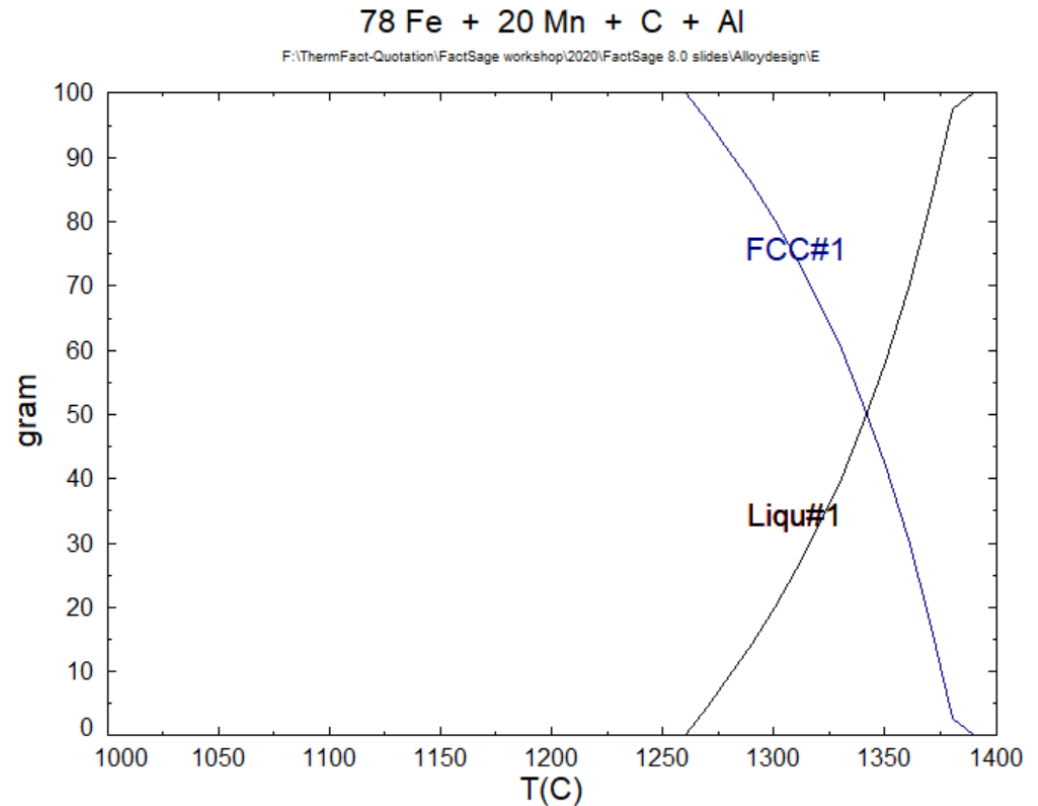
+ 0 gram BCC_B2#1
+ 0 gram BCC_B2#2
(1400 C, 1 atm, a=0.94610)
( 3.5787E-02 wt.% Al1Al1Va6
+ 1.6883 wt.% Al1Fe1Va6
+ 0.28845 wt.% Al1Mn1Va6
+ 1.6883 wt.% Fe1Al1Va6
+ 69.977 wt.% Fe1Fe1Va6
+ 11.990 wt.% Fe1Mn1Va6
+ 0.28845 wt.% Mn1Al1Va6
+ 11.990 wt.% Mn1Fe1Va6
+ 2.0542 wt.% Mn1Mn1Va6)

+ 0 gram CUB_Al3
(1400 C, 1 atm, a=0.81702)
( 1.2558E-03 wt.% AlC
+ 0.82079 wt.% AlVa
+ 9.9046E-02 wt.% FeC
+ 76.997 wt.% FeVa
+ 2.8451E-02 wt.% MnC
    
```

Final Conditions	T(C)	P(atm)	Product H(J)
<A>	1400	600	10

81 calculations

Calculate >>



Scheil cooling solidification of steel: TWIP steel

Scheil cooling of Fe-20Mn-1C-1Al TWIP steel

Equilib - Menu: File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 78 Fe + 20 Mn + C + Al

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 33

species: 33

Scheil-Gulliver cooling

FSstel-Liqu Options

Cooling step: 5 T-auto:

Quantity(g): 0

Legend

L - immiscible 6

L - Scheil cooling

+ - selected 10

Show all selected

species: 108

solutions: 22

Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1400	1	

10 steps Table

Scheil-Gulliver cooling - T(start) = 1400, T(stop) = 0

Equilibrium

normal normal

transitions only

- no time limit - C

*	+	Base-Phase	Full Name
	IL	FSstel-Liqu	LIQUID
	I	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FSstel-HCP	HCP_A3
	+	FSstel-CEME	CEMENTITE
	+	FSstel-M23C	M23C6
	+	FSstel-M7C3	M7C3
	+	FSstel-CBCC	CBCC_A12

Custom Solutions

fixed activities

ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties

apply back diffusion

Virtual species:

Total Species (max)

Total Solutions (max)

Total Phases (max)

Scheil-Gulliver cooling



In Scheil-Gulliver cooling it is not permitted to select option 'J' (i.e. possible 3-phase immiscibility) for a solution phase - for example FSstel-FCC

In the 'Solution phases' frame click on 'Select' and then select 'Change all [J] to [I] (3-phase to 2-phase)'.

OK

Scheil-Gulliver cooling



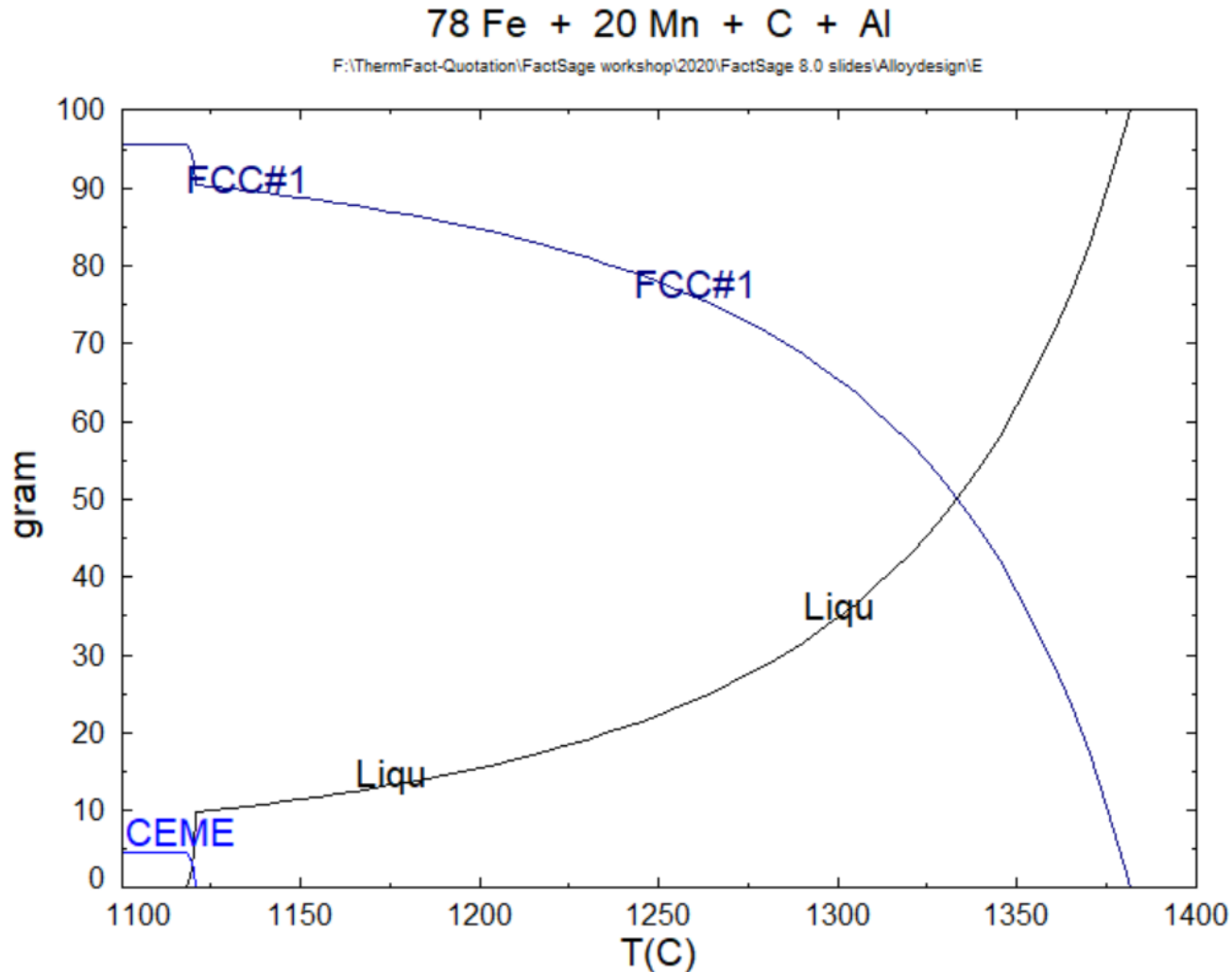
In Scheil-Gulliver cooling it is not permitted to select an ordered phase - BCC_B2!BCC_A2

In the 'Solution phases' frame remove FSstel-BCC2 from the phase selection.

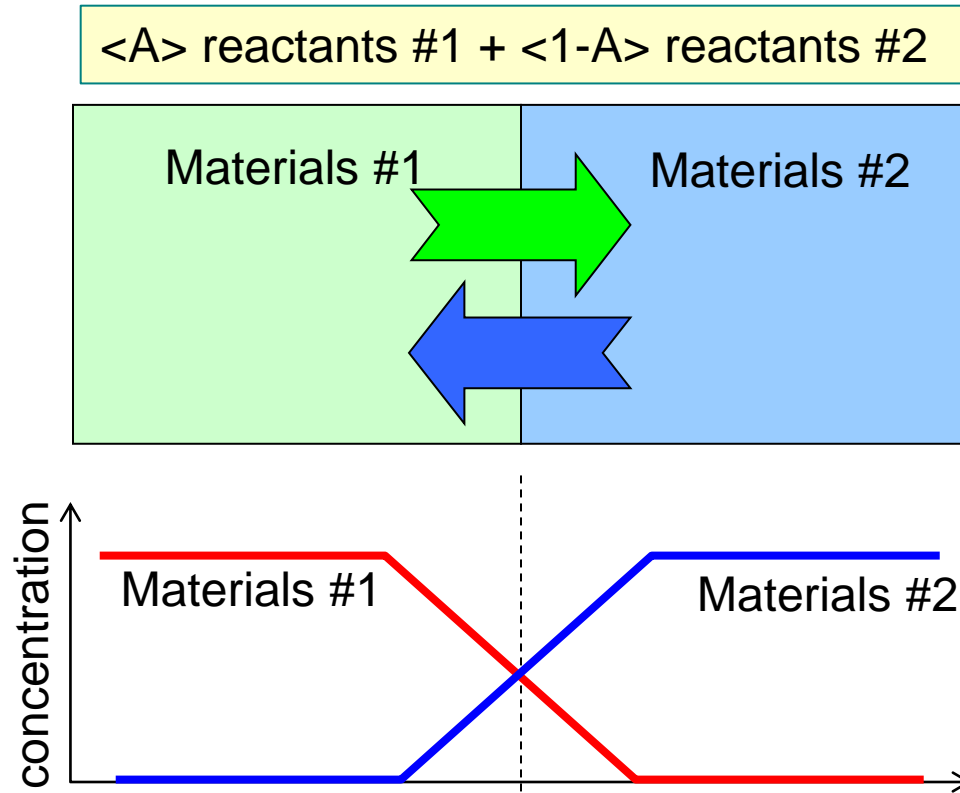
OK

Scheil solidification of steel: TWIP steel

Solidification is completed at $\sim 1116^\circ\text{C}$ which is almost 150°C lower than equilibrium calculation.

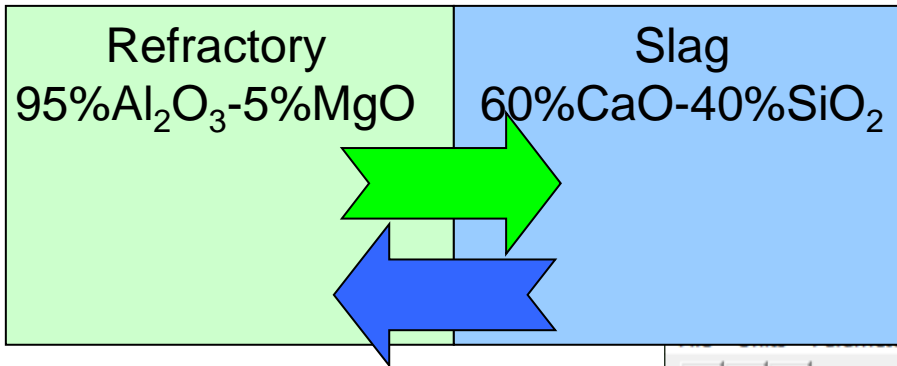


Simple counter-cross inter-diffusion calculation: <A> option



Counter-cross inter-diffusion reactions at interface can be simulated with the <A> option in Equilib. This assumes the diffusivities of all components in both materials are the same.

Counter-cross reaction: refractory / slag



system

rs Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) <0.6A> CaO + <0.4A> SiO2 + <0.95-0.95A> Al2O3 + <0.05-0.05A> MgO

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 50

species: 50

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,

Legend

| - immiscible 5

+ - selected 9

Show all selected

species: 82

solutions: 19

Select

Custom Solutions

0 fixed activities [Details ...](#)

0 ideal solutions

Pseudonyms

apply [Edit ...](#)

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin [edit](#)

Virtual species: 12

Total Species (max 5000) 132

Total Solutions (max 200) 19

Total Phases (max 1500) 69

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0	1	1600	1	

10 steps Table

101 calculations

Equilibrium

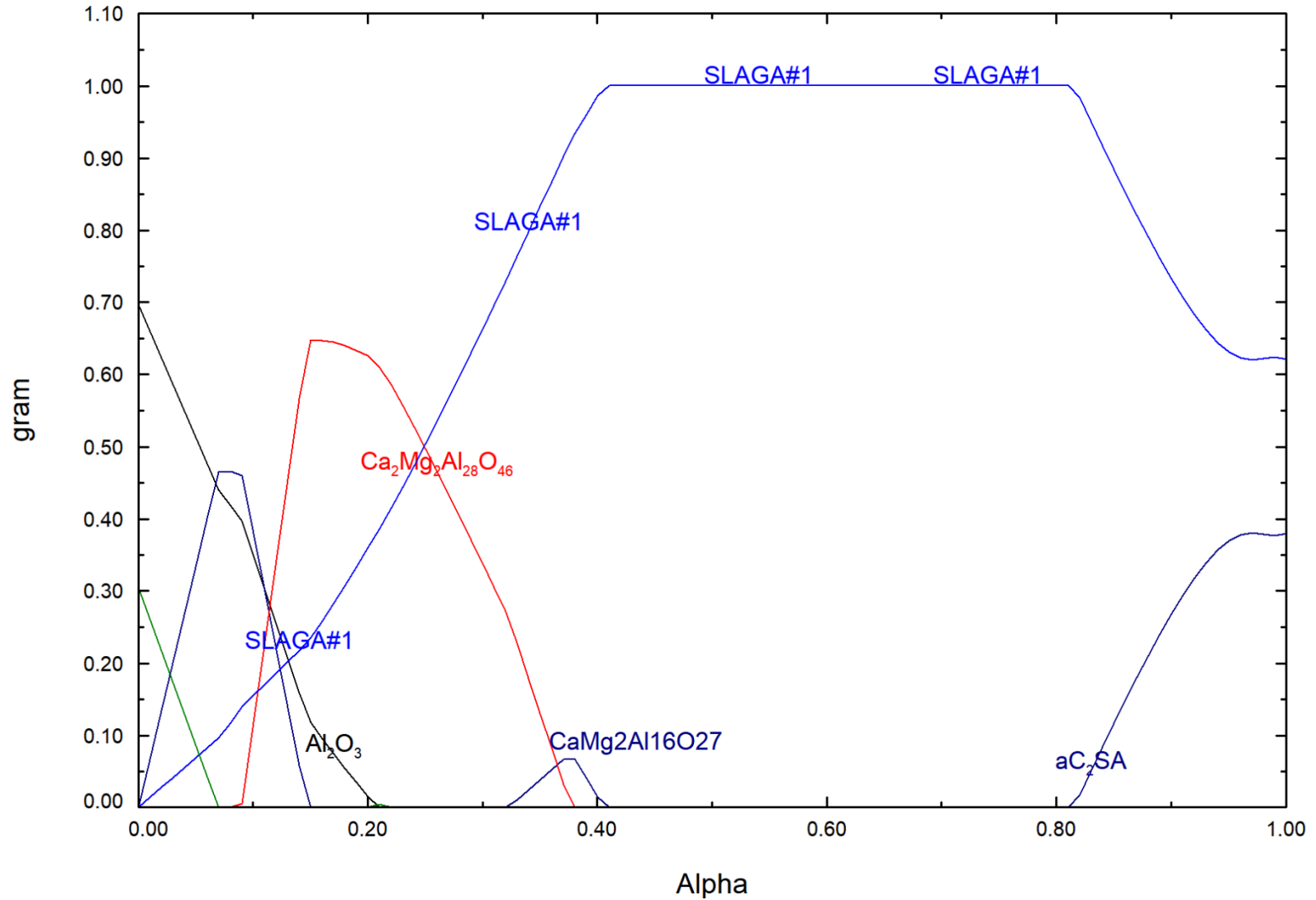
normal normal + transitions

transitions only open

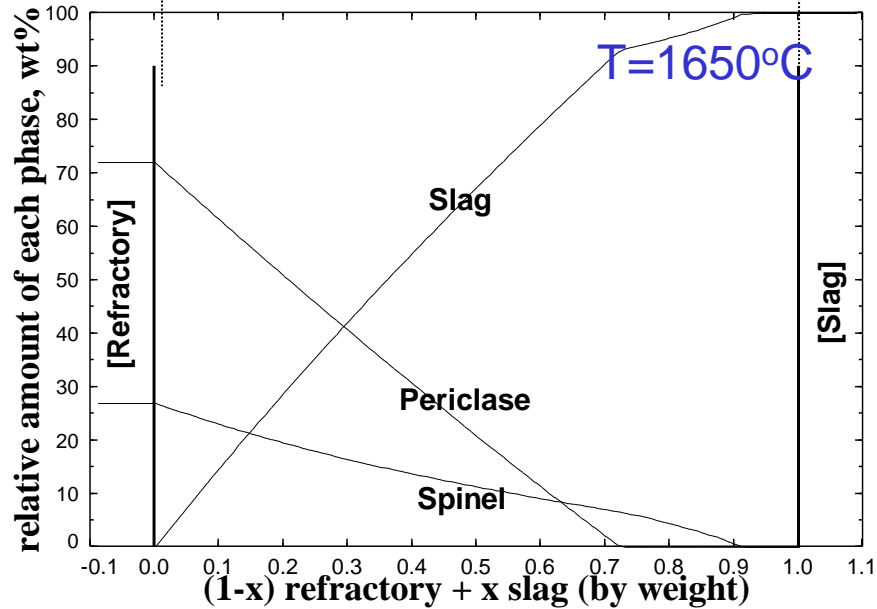
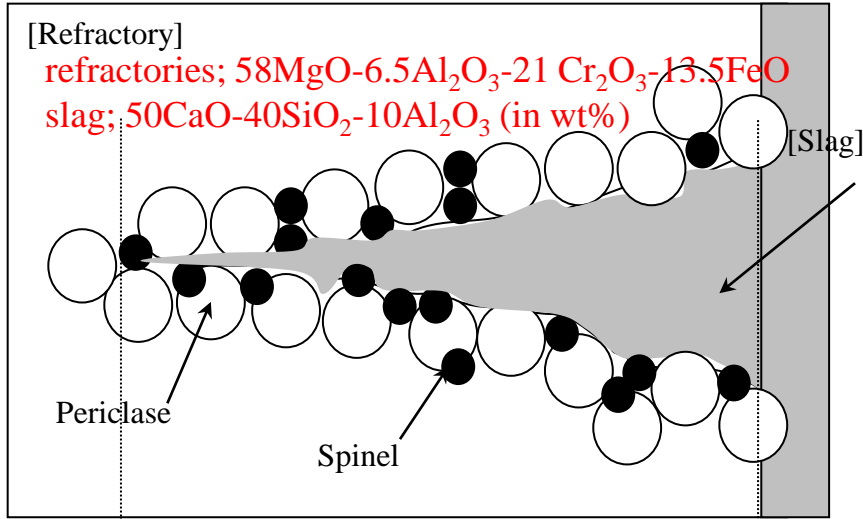
- no time limit - [Calculate >>](#)

FactSage 8.0

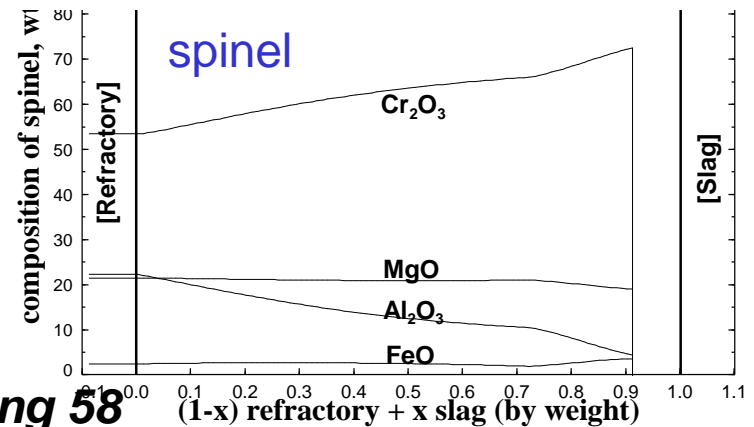
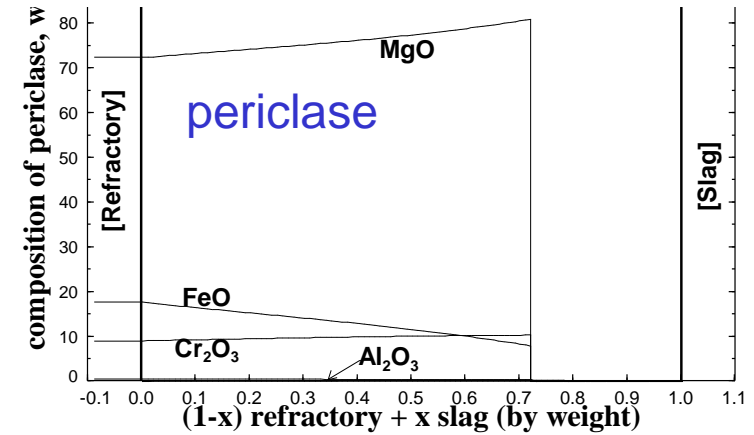
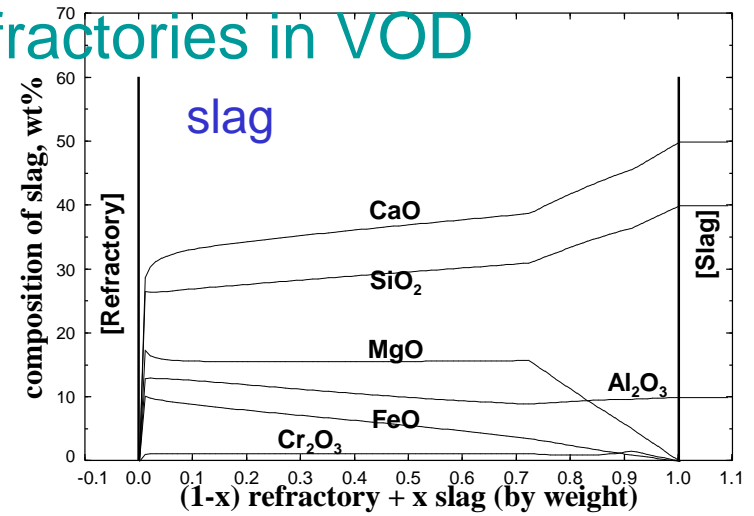
Counter-cross reaction: refractory / slag



Counter-cross reaction: Refractories in VOD



Jung et al., Taikabutsu, vol. 56, 2004, pp. 382-386.



Application: Activity calculations

Slag: binary, ternary and multi-component systems
FeLq : oxygen and alloying elements

Now in FactSage 70, iso-activity lines in ternary or higher order system can be easily calculated using Phase Diagram module

Activity calculations – Binary system

Equilib - Menu:

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(gram) <1-A> CaO + <A> SiO2

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 16

species: 16

Solution phases

*	+	Base-Phase	Full Name
I		FToxid-SLAGA	A-Slag-liq all oxides + S

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

Target

Estimate T(K): 1000

Quantity(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.1	0.01	1600	1	

10 steps Table 101 calculations

FactSage 8.0

Axes: activity vs Alpha

Y-variable X-variable Swap Axes

Y-axis

activity

maximum 1

minimum 0

tick every 0.1

X-axis

Alpha

maximum 1

minimum 0

tick every 0.1

Cancel Refresh OK

Plot Species Selection - Equilib Results: activity vs Alpha

File Show Select

+	#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	Activity (max)
	3	SiO2	0	0	0	100	0	0.962847
	4	CaO	0	0	0	100	0	0.174852
	Pure Liquids							
+	5	SiO2	0	0	0	0	0	0.962846
	6	CaO	0	0	0	0	0	0.174852
	Pure Solids							
	7	SiO2	0	0	0	0	0	0.110411
	8	SiO2	0	0	0	0	0	0.908572
	9	SiO2	0	0	0	0	0	2.1743E-03
	10	SiO2	0	0	0	0	0	0.999329
	11	SiO2	0	0	0	0	0	1.0954E-02
+	12	SiO2	0	1	0	0	0	1
	13	SiO2	0	0	0	0	0	0.430937
	14	SiO2	0	0	0	0	0	9.5779E-03
+	15	CaO	0	1	0	0	0	1
	16	CaSiO3	0	0	0	0	0	0.749399
	17	CaSiO3	0	0	0	0	0	0.887701
	18	Ca2SiO4	0	0	0	0	0	0.206145

Display

source

phase

name

[page]

Mass

mole

gram

Order

integer #

mass (max)

fraction (max)

activity (max)

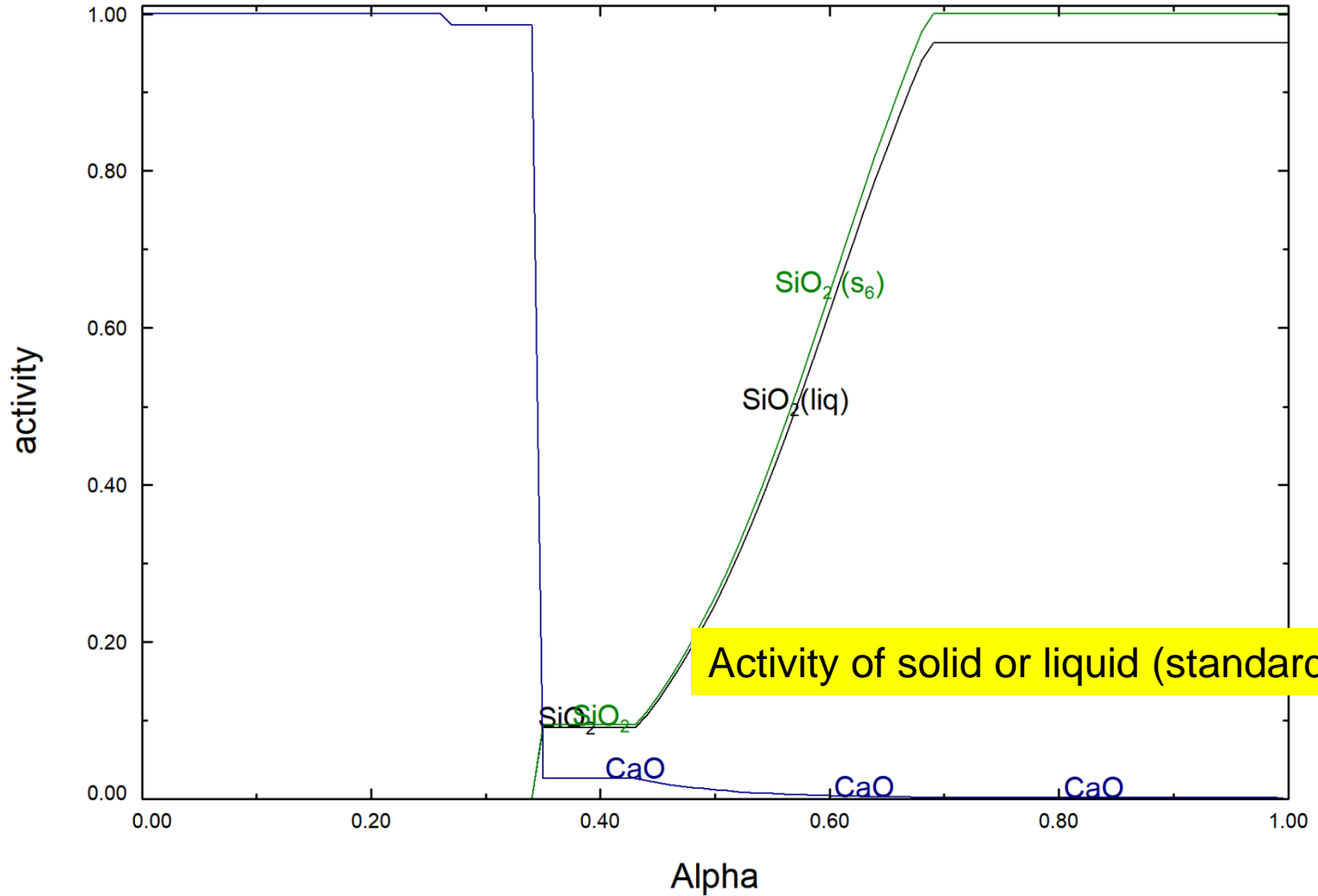
Select Top 15 3 species selected

ignore species and phases with zero mass

Select ... OK

Click on the '+' column to add or remove species. 101 pages

Activity calculations – Binary system



Activity of solid or liquid (standard state) ?

Activity calculations – Ternary system

Calculation of iso-activity line of $\text{SiO}_2(\text{s6})$ in the CaO-MgO-SiO_2 system

The screenshot shows the FactSage 8.1 interface. The main window is titled "Phase Diagram - Menu: last system". The components list includes CaO, MgO, and SiO2. The products list includes various SiO2 polymorphs and silicates. The variables section shows T(C) set to 1600, SiO2/(CaO) set to 0.1, and MgO/(CaO) set to 0.1. The "Selection - Phase Diagram" window is open, showing a list of phases with "SiO2(s6)" selected. A yellow box highlights the "SiO2(s6)" entry in the selection list.

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	4	MgO(s)	FToxid	periclase	V				
+	5	SiO2(s)	FToxid	Quartz(l)	V				
+	6	SiO2(s2)	FToxid	Quartz(h)	V				
+	7	SiO2(s3)	FToxid	Tridymite(l)	V				
(2)		SiO2(s4)	FToxid	Tridymite(h)	V				
(2)		SiO2(s5)	FToxid	Cristobalite(l)	V				
		SiO2(s6)	FToxid	Cristobalite(h)	V				
+	11	SiO2(s7)	FToxid	coesite	V				
+	12	SiO2(s8)	FToxid	stishovite	V				
+	13	MgSiO3(s)	FToxid	low-clinoenstatite	V				
+	14	MgSiO3(s2)	FToxid	ortho-enstatite	V				
+	15	MgSiO3(s3)	FToxid	proto-enstatite	V				
+	16	MgSiO3(s4)	FToxid	high-P-clinoenst.	V				
+	17	MgSiO3(s5)	FToxid	Mg-ilmenite	V				
+	18	MgSiO3(s6)	FToxid	Mg-garnet	V				
+	19	MgSiO3(s7)	FToxid	Mg-perovskite	V				
+	20	Mg2SiO4(s)	FToxid	forsterite	V				
+	21	Mg2SiO4(s2)	FToxid	beta-forsterite	V				
+	22	Mg2SiO4(s3)	FToxid	gamma-forsterite	V				
+	23	CaO(s)	FToxid	Lime	V				
+	24	CaSiO3(s)	FToxid	Wollastonite	V				

(1) Run phase diagram and select the axis and temperature.

(2) Click the solid or liquid phase you want to set its activity. For example, select "SiO2(s6)" in this example

Activity calculations – Ternary system

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 30/30 **SOLID**

+	Code	Species	Data
+	4	MgO(s)	FToxid p
+	5	SiO2(s)	FToxid Q
+	6	SiO2(s2)	FToxid Q
+	7	SiO2(s3)	FToxid T
+	8	SiO2(s4)	FToxid T
+	9	SiO2(s5)	FToxid C
+	10	SiO2(s6)	FToxid C
+	11	SiO2(s7)	FToxid c
+	12	SiO2(s8)	FToxid st
+	13	MgSiO3(s)	FToxid lo
+	14	MgSiO3(s2)	FToxid oi
+	15	MgSiO3(s3)	FToxid pi
+	16	MgSiO3(s4)	FToxid hi
+	17	MgSiO3(s5)	FToxid M
+	18	MgSiO3(s6)	FToxid M
+	19	MgSiO3(s7)	F
+	20	Mg2SiO4(s)	F
+	21	Mg2SiO4(s2)	F
+	22	Mg2SiO4(s3)	FToxid g
+	23	CaO(s)	FToxid Lime
+	24	CaSiO3(s)	FToxid Wollastonite

10 SiO2(s6)

- clear

+ - select

- standard stable phase

! - dormant (metastable) phase

F - formation target phase

P - precipitate target phase

16

L - cooling calculation ...

Ideal Solution

Z - iso-activities ...

Help ...

permit selection of 'X' species Help Suppress Duplicates Edit priority list

Show Selected Select All Select/Clear... Clear

Iso-activity lines of SiO2(s6)

Enter up to 10 iso-activities for SiO2(s6)

Enter 0 or Click on [Cancel] to delete the values.

OK

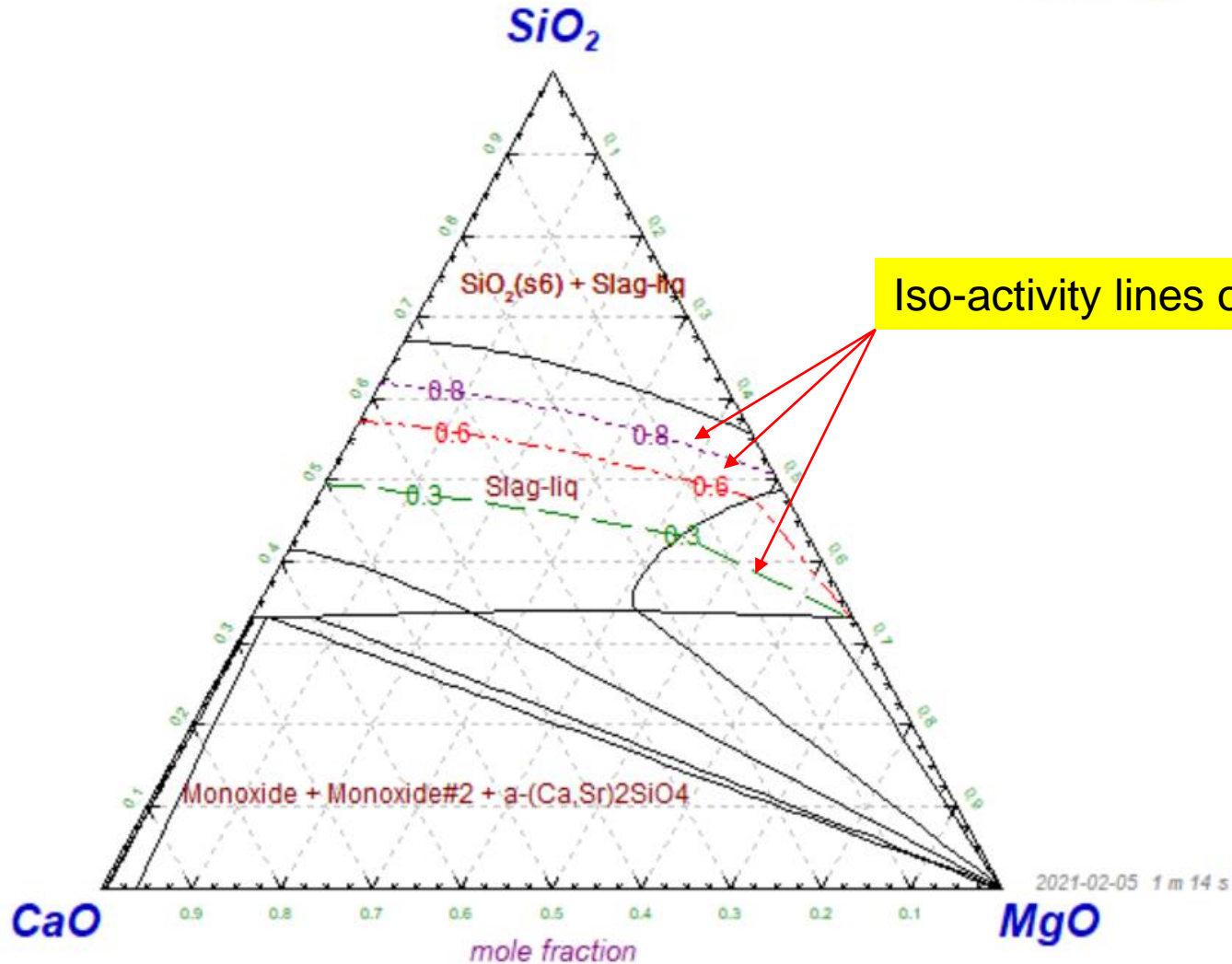
Cancel

0.3 0.6 0.8

- (2) Click the solid or liquid phase you want to set its activity. For example, select “liquid Mg” in this example
- (3) Click “Z - iso-activities”
- (4) Set the activity values to plot in phase diagram – up to 10 values

Activity calculations – Ternary system

CaO - MgO - SiO₂
1600°C, 1 atm, SiO₂(s6) iso-activities



Activity calculations – Quaternary or higher order system

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 50/50 **SOLID**

Iso-activity lines of SiO2(s6)

Enter up to 10 iso-activities for SiO2(s6)

Enter 0 or Click on [Cancel] to delete the values.

0.30608

OK Cancel

Code	Species	Data	P
+ 5	MgO(s)	FToxid	pericl
+ 6	Al2O3(s)	FToxid	gamm
+ 7	Al2O3(s2)	FToxid	delta
+ 8	Al2O3(s3)	FToxid	kappa
+ 9	Al2O3(s4)	FToxid	corun
+ 10	SiO2(s)	FToxid	Quartz
+ 11	SiO2(s2)	FToxid	Quartz(h)
+ 12	SiO2(s3)	FToxid	Tridymite(l)
+ 13	SiO2(s4)	FToxid	Tridymite(h)
+ 14	SiO2(s5)	FToxid	Cristobalite(l)
+ 15	SiO2(s6)	FToxid	Cristobalite(h)
+ 16	SiO2(s7)	FToxid	coesite
+ 17	SiO2(s8)	FToxid	stishovite
+ 18	MgSiO3(s)	FToxid	low-clinoenstatite
+ 19	MgSiO3(s2)	FToxid	ortho-enstatite
+ 20	MgSiO3(s3)	FToxid	proto-enstatite
+ 21	MgSiO3(s4)	FToxid	high-P-clinoenst.
+ 22	MgSiO3(s5)	FToxid	Mg-ilmenite
+ 23	MgSiO3(s6)	FToxid	Mg-garnet
+ 24	MgSiO3(s7)	FToxid	Mg-perovskite
+ 25	Mg2SiO4(s)	FToxid	forsterite

permit selection of '*' species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

pure liquids
 pure solids
 species: 50

Formation Target
 SiO2(s6)
 Estimate T(K): 1000

Legend
 I - immiscible 5
 + - selected 9

Show all selected
 species: 82
 solutions: 19 **Select**

Variables

T(C)	SiO2/(CaO)	MgO/(CaO)	Al2O3/(CaO)
1600	0.1	0.1	0.05 (min)

 A = SiO2, B = CaO, C = MgO

Solution phases

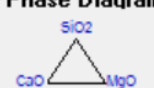
*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	I	FToxid-MeO_A	A-Monoxide
	I	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,

Custom Solutions
 SiO2(s6) iso-activity **Details ...**

Pseudonyms
 apply **Edit ...**

Volume and physical prop data
 assume molar volumes of solids and liquids = 0
 use only molar volume data
 use V & phys. property data

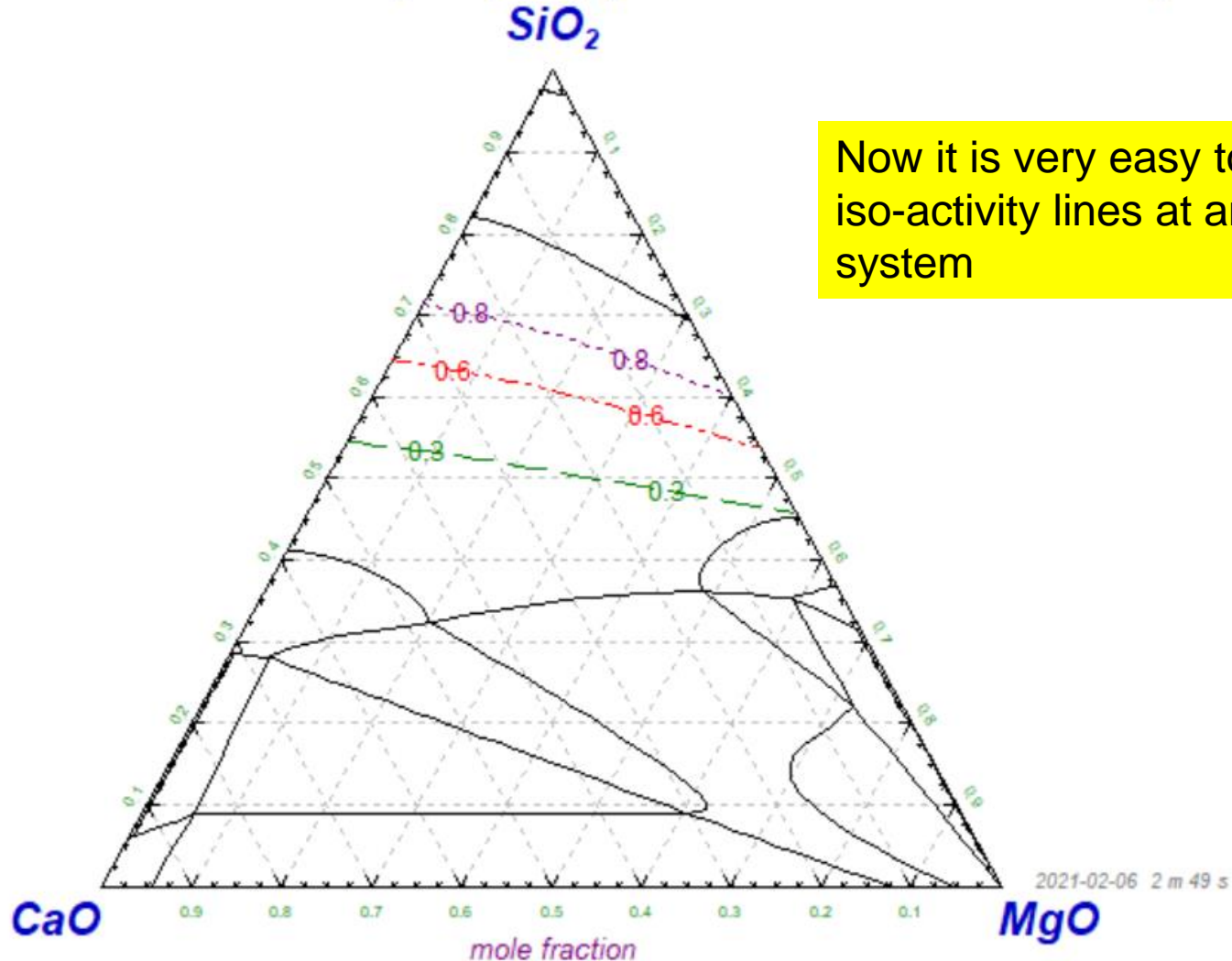
paraequilibrium & Gmin **edit**
 Virtual species: 12
Total Species (max 5000) 132
Total Solutions (max 200) 19
Total Phases (max 1500) 69

Phase Diagram

 - no time limit - **Calculate >>**

FactSage 8.1

Activity calculations – Quaternary or higher order system

CaO - MgO - SiO₂ - Al₂O₃
 $Al_2O_3/(CaO+MgO+SiO_2+Al_2O_3)(mol/mol)=0.05,$
1600 C, 1 atm, SiO₂(s6) iso-activities



Now it is very easy to calculate iso-activity lines at any high order system

Activity of oxygen (wt% standard state) in liquid steel

$$RT \ln \gamma_M^o = g_M^o(\text{Henrian S.S.}) - g_M^o(\text{Pure Element S.S.})$$

$$\Rightarrow a_{M(\text{pure Element S.S.})} = \gamma_M^o a_{M(\text{Henrian s.s.})}$$

$a_{\text{O in FeLq}}$

$\ln \gamma_{\text{O}}^o = -15280/T + 3.5$: value used in FeLq database; slightly different depending on assessments

Reference pure element standard state of O in FeLq : Gas (0.5 O₂)

$$a_i(\text{wt\% std. state}) = \frac{100M_i}{M_{\text{Fe}}} a_i(\text{Henrian std. state})$$

$$\text{Log } a_{\text{O}(\text{wt\%})} = \text{Log}(a_{\text{O in FeLq}}) - \text{Log}((\text{EXP}(-15280/T+3.5)*55.847/100/16))$$

where T in Kelvin

Activity of oxygen (wt% standard state) in liquid steel

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (3)

(gram) 99.95 Fe + <A> Al + 0.05 O

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 8

species: 8

Target: none

Estimate T(K): 1000

Quantity(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.6	0.01	1600	1	

10 steps Table 61 calculations

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-CORU	M2O3(Corundum)

Legend: + selected 1

Show: all selected

species: 5

solutions: 1 Select

Equilibrium

normal normal + transitions

transitions only open

- no time limit - Calculate >>

FactSage 8.0

Equilib - Results A=0.1 (page 11/61)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

A=0.13 | A=0.14 | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24

A=0 | A=0.01 | A=0.02 | A=0.03 | A=0.04 | A=0.05 | A=0.06 | A=0.07 | A=0.08 | A=0.09 | -A=0.1 | -A=0.11 | A=0.12

(gram) 99.95 Fe + <A> Al + 0.05 O =

99.995 gram Fe-liq
(99.995 gram, 1.7914 mol)
(1600 C, 1 atm, a=1.0000)
(99.955 wt.% Fe
+ 4.3874E-02 wt.% Al
+ 2.2061E-04 wt.% O
+ 5.7583E-04 wt.% AlO
+ 8.2991E-05 wt.% Al2O)

System component

System component	Amount/mol
Fe	1.7898
Al	1.6417E-03
O	2.8371E-05

Total dissolved Al and O

Dissolved Al, O, Al*O, Al2*O

PHASE: Fe-liq	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
gram			
Fe	9.9950E+01	9.9955E-01	9.9908E-01
Al	4.3871E-02	4.3874E-04	5.2325E-05
O	2.2060E-04	2.2061E-06	7.3052E-08
AlO	5.7580E-04	5.7583E-06	7.4782E-06
Al2O	8.2987E-05	8.2991E-07	6.6213E-07
TOTAL:	9.9995E+01	1.0000E+00	1.0000E+00

a_O in FeLq

System component	Amount/mol	Amount/g	Mole fraction	Mass fraction
Fe	1.7898	99.950	0.99907	0.99955
Al	1.6417E-03	4.4297E-02	9.1643E-04	4.4299E-04
O	2.8371E-05	4.5392E-04	1.5837E-05	4.5394E-06

ACTIVITY

System component	Amount/mol	Amount/g	Mole fraction	Mass fraction
Fe	1.7898	99.950	0.99907	0.99955
Al	1.6417E-03	4.4297E-02	9.1643E-04	4.4299E-04
O	2.8371E-05	4.5392E-04	1.5837E-05	4.5394E-06

ACTIVITY

System component	Amount/mol	Amount/g	Mole fraction	Mass fraction
Fe	1.7898	99.950	0.99907	0.99955
Al	1.6417E-03	4.4297E-02	9.1643E-04	4.4299E-04
O	2.8371E-05	4.5392E-04	1.5837E-05	4.5394E-06

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.6	0.01	1600	1	

61 calculations Calculate >>

Activity of oxygen (wt% standard state) in liquid steel

Equilib - Results A=0.1 (page 11/61)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

A=0.13 A=0.14 A=0.15 A=0.16 A=0.17 A=0.18 A=0.19 A=0.2 A=0.21 A=0.22 A=0.23 A=0.24

A=0 A=0.01 A=0.02 A=0.03 A=0.04 A=0.05 A=0.06 A=0.07 A=0.08 A=0.09 A=0.1 A=0.11 A=0.12

(gram) 99.95 Fe + <A> Al + 0.05 O =

99.995 gram Fe-11q

Spreadsheet Setup

System Properties

Property columns 1 - 1 -

Column: - 1 -

Variable: Alpha

Species Properties

Columns per species 2 - 1 - - 2 -

order species order props.

Column: - 1 - - 2 -

Variable: Wt% a

Species

Columns: 5

Select ...

Cancel

Default

Selected: 2

Spreadsheet - Equilib Page 11/61 : T(C) = 1600, P(atm) = 1, Alpha = 0.1

File Edit Show Select Stable

Selected: 2/15

Spreadsheet Species

Page 11/61 : T(C) = 1600, P(atm) = 1, Alpha = 0.1 [min = 0 at p. 1; max = 0.6 at p.

+	Code	Species	Data	Phase	T	V	Activity	Minimum
	2	Al2O3(s)	FToxid	gamma	V	0.6513	0 [1]	
	3	Al2O3(s2)	FToxid	delta	V	0.7993	0 [1]	
	4	Al2O3(s3)	FToxid	kappa	V	0.7818	0 [1]	
	5	Al2O3(s4)	FToxid	corundum(alpha)	V	1.000	0 [1]	
	6	Fe2O3(s)	FToxid	hematite	V	2.0193E-12	1.2577E-14 [61]	
	7	Fe2O3(s2)	FToxid	High-Pressure-H	V	1.3537E-14	8.4315E-17 [61]	
	8	Fe2O3(s3)	FToxid	High-Pressure-H	V	1.4655E-14	9.1278E-17 [61]	
	9	Al2Fe2O6(s)	FToxid	solid	o	4.3995E-12	0 [1]	
	10	Fe(FeLq)	FTmisc	FTmisc-FeLq		0.9991	0.9887 [61]	
	11	Al(FeLq)	FTmisc	FTmisc-FeLq		5.2325E-05	0 [1]	
+	12	O(FeLq)	FTmisc	FTmisc-FeLq		7.3052E-08	1.3534E-08 [61]	
	13	AlO(FeLq)	FTmisc	FTmisc-FeLq		7.4782E-06	0 [1]	
	14	Al2O(FeLq)	FTmisc	FTmisc-FeLq		6.6213E-07	0 [1]	
	50	Solution	FTmisc	FTmisc-FeLq		1.000	1.000	
+	59	All Elements	FTmisc	FTmisc-FeLq				1.000

* denotes all the Species Properties as defined in the Spreadsheet Setup.

Select All Clear OK

a_O in FeLq

Total dissolved Al and O

A	B	C	D	E	F
Alpha	Wt%-O(FeLq)	a-O(FeLq)	Wt%-Fe_FTmisc-FeLq	Wt%-Al_FTmisc-FeLq	Wt%-O_FTmisc-FeLq
0	0.05	1.65438E-05	99.95	0	0.05
0.01	0.041132225	1.36127E-05	99.958808	4.37926E-05	0.041147937
0.02	0.032247443	1.06746E-05	99.96768	5.48179E-05	0.032265182
		3722E-06	99.976535	7.54777E-05	0.023389413

Dissolved unassociated O

A	B	C	D	E	F	G	H	I	J
1	Alpha	Wt%-O(FeLq)	a-O(FeLq)	Wt%-Fe_FTmisc-FeLq	Wt%-Al_FTmisc-FeLq	Wt%-O_FTmisc-FeLq	a-Fe_FTmisc-FeLq	a-Al_FTmisc-FeLq	a-O_FTmisc-FeLq
2	0	0.05	1.65438E-05	99.95	0	0.05	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
3	0.01	0.041132225	1.36127E-05	99.958808	4.37926E-05	0.041147937	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
4	0.02	0.032247443	1.06746E-05	99.96768	5.48179E-05	0.032265182	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
5	0.03	0.023368581	7.73722E-06	99.976535	7.54777E-05	0.023389413	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
6	0.04	0.014513047	4.80625E-06	99.985334	0.00012696	0.014539475	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
7	0.05	0.005837232	1.93351E-06	99.993728	0.000393134	0.00587891	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
8	0.06	0.000963527	3.1918E-07	99.993945	0.004987647	0.001067027	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
9	0.07	0.000467675	1.54909E-07	99.984894	0.014487143	0.000619046	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
10	0.08	0.000329524	1.09138E-07	99.975117	0.024369484	0.000513357	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
11	0.09	0.00026181	8.67022E-08	99.965206	0.034322168	0.000472016	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
12	0.1	0.000220614	7.30519E-08	99.955247	0.044299009	0.000453944	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
13	0.11	0.0001925	6.37357E-08	99.945267	0.054286291	0.000446942	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
14	0.12	0.000171891	5.6906E-08	99.935275	0.064278482	0.000446089	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
15	0.13	0.000156026	5.16482E-08	99.925278	0.074272916	0.000449013	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
16	0.14	0.00014337	4.7454E-08	99.915277	0.084268152	0.000454433	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
17	0.15	0.000132999	4.40165E-08	99.905275	0.094263343	0.000461593	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
18	0.16	0.000124317	4.11386E-08	99.895272	0.10425796	0.000470022	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
19	0.17	0.000116923	3.86877E-08	99.885269	0.11425165	0.00047941	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
20	0.18	0.000110536	3.65706E-08	99.875266	0.12424418	0.000489544	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
21	0.19	0.000104955	3.47201E-08	99.865264	0.13423538	0.000500274	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->
22	0.2	0.000100000	3.29000E-08	99.855263	0.14422610	0.000511100	<-not-calcd.->	<-not-calcd.->	<-not-calcd.->

→ Then, convert a_O in FeLq to a_O wt% s.s.

Thermodynamic properties: ΔG , ΔH , ΔS etc.

For calculating the difference of thermodynamic properties from the initial state to the final state, "Initial Conditions" should be activated.

Initial conditions for phase and temperature should be specified

** P(total) is the hydrostatic pressure above the phase.
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Initial Conditions

Next >>

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S

Legend

I - immiscible 1

Show all selected

species: 4

solutions: 2

Select

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0	1	0.01	1600	1

10 steps Table 101 calculations

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Edit ...

Volume data

assume molar volumes of

solids and liquids = 0

include molar volume data

and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 4

Total Solutions (max 200) 2

Total Phases (max 1500) 2

Equilibrium

normal normal + transitions

transitions only open

- no time limit - Calculate >>

Thermodynamic properties: Activity, ΔG , ΔH , ΔS etc.

Plot: Delta G(J) vs Alpha

File Help

<1-A> CaO + <1A> SiO2

Axes	Variables	Minimum	Maximum
	activity	0	1
	mole	0	2
	mole fract. soln. species	0	1
	gram	0	60.084
	weight % soln. species	0	100
X-axis	Alpha	0	1
	T(C)	1600	1600
	P(atm)	1	1
	Delta Cp(J/K)	-2.9405E-05	34.285
Y-axis	Delta G(J)	-6.5998E+04	0
	Vol(litre)	0	0
	Delta H(J)	-8.0060E+04	273.19
	Delta V(litre)	0	0
	Delta S(J/K)	-7.8495	7.2123
	- page -	1	101

Axes Species: 0 selected

Delta G(J) vs Alpha

Buttons: Select, Axes, Repeat

Graph

Labels: size: 9 no: 4

Display:

- color
- full screen
- reactants
- Viewer
- file name
- Figure

Buttons: Plot >>

FactSage 8.0 | C:\Workshop80\Myresult\Equi0.res | 24Dec19 | 101 sets

Axes: Delta G(J) vs Alpha

Y-variable X-variable Swap Axes

Y-axis: Delta G(J)

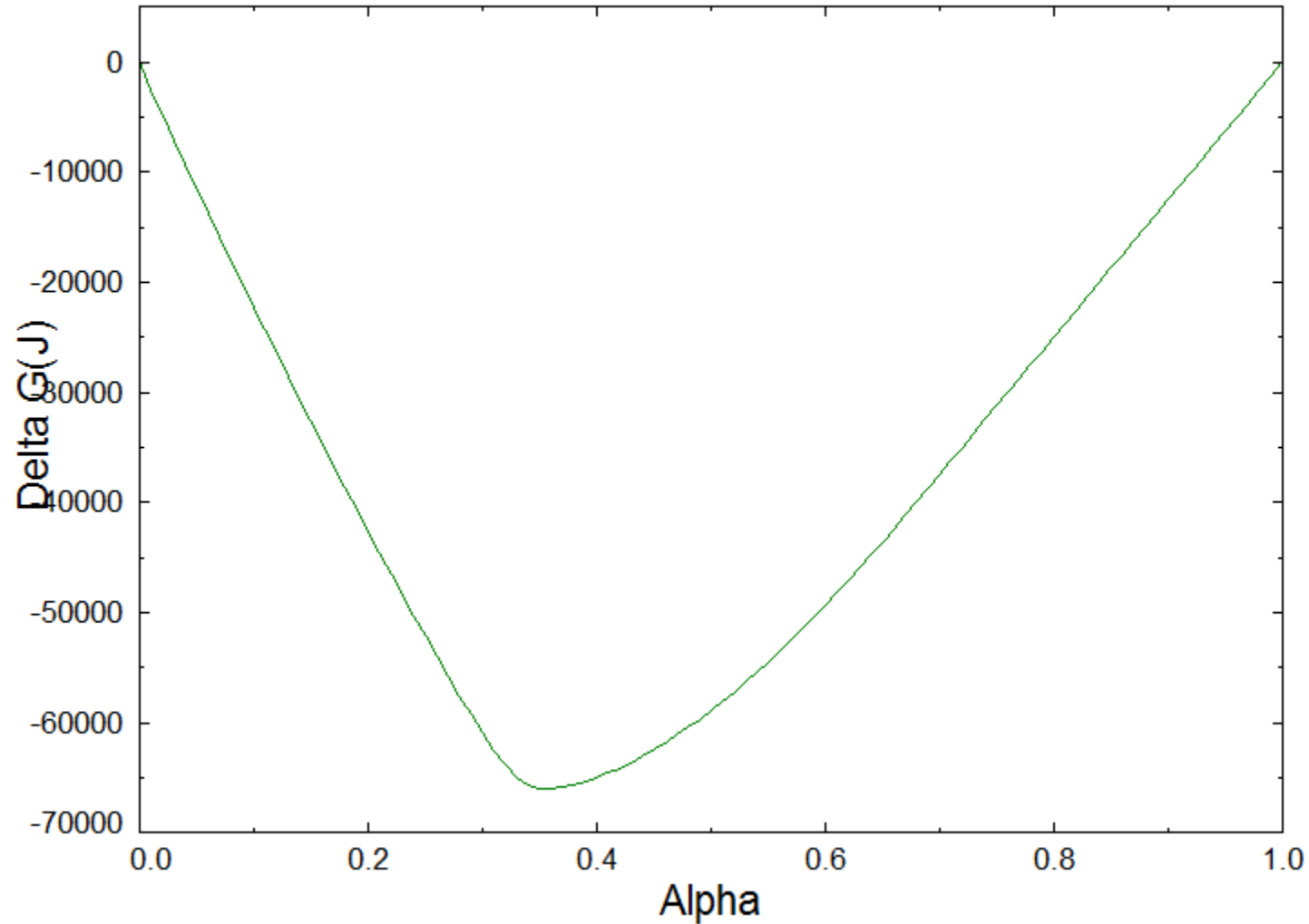
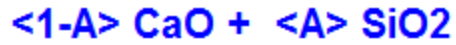
maximum: 0
minimum: -70000
tick every: 5000

X-axis: Alpha

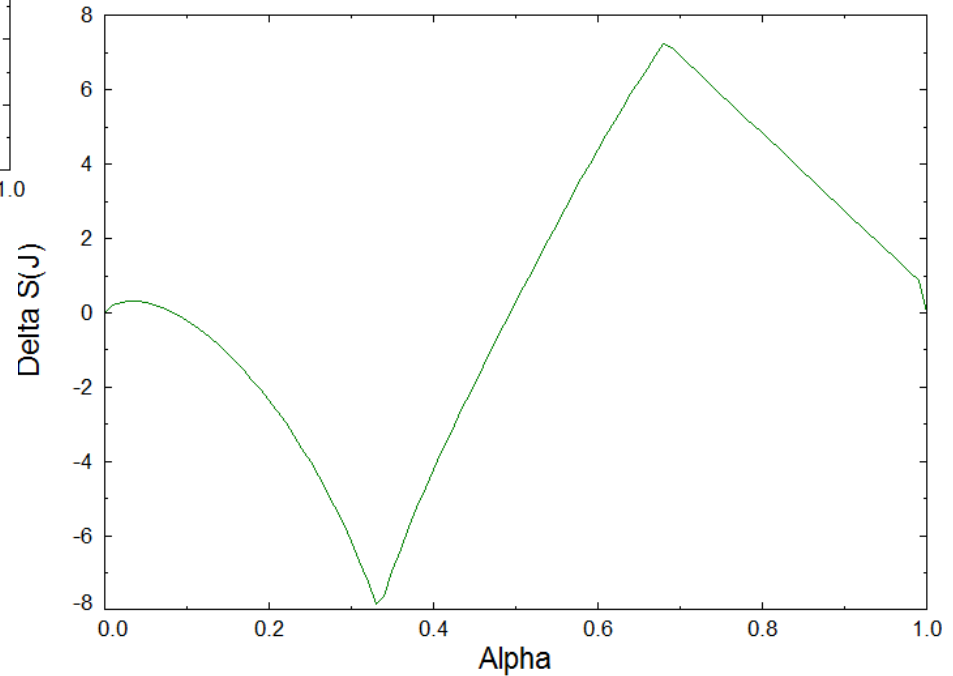
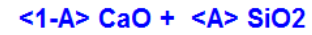
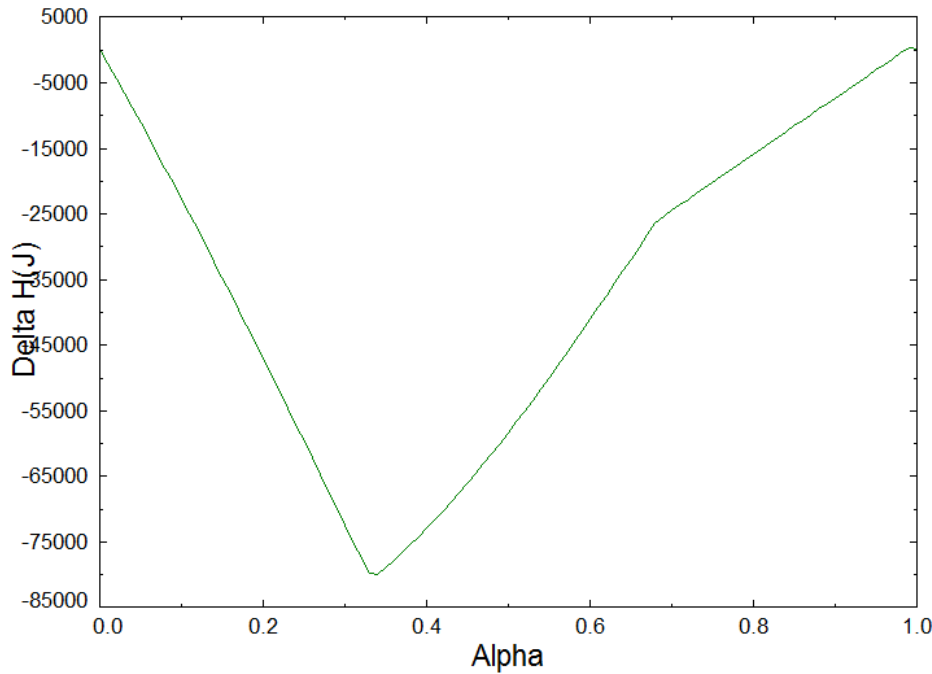
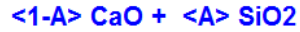
maximum: 1
minimum: 0
tick every: 0.1

Buttons: Cancel, Refresh, OK

Thermodynamic properties: ΔG , ΔH , ΔS etc.



Thermodynamic properties: Activity, ΔG , ΔH , ΔS etc.



Simple examples of Phase diagram

Binary phase diagram
Ternary and multi-component systems

Binary phase diagram: CaO-SiO₂

There is a stable miscibility gap in slag; automatic selection by FactSage

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (2)

(gram) CaO + SiO₂

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 16

species: 16

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	I	FToxid-SLAGA
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		A-Slag-liq all oxides + S

Legend

I - immiscible 1

Show all selected

species: 4

solutions: 2

Select

Custom Solutions

0 fixed activities

0 ideal solutions

Details ...

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 2

Total Species (max 5000) 20

Total Solutions (max 200) 2

Total Phases (max 1500) 18

Variables

T(C)	100SiO ₂ /(CaO)			
1000 2000	0 100			

T(C) vs 100SiO₂/(CaO+SiO₂)

Phase Diagram

Y

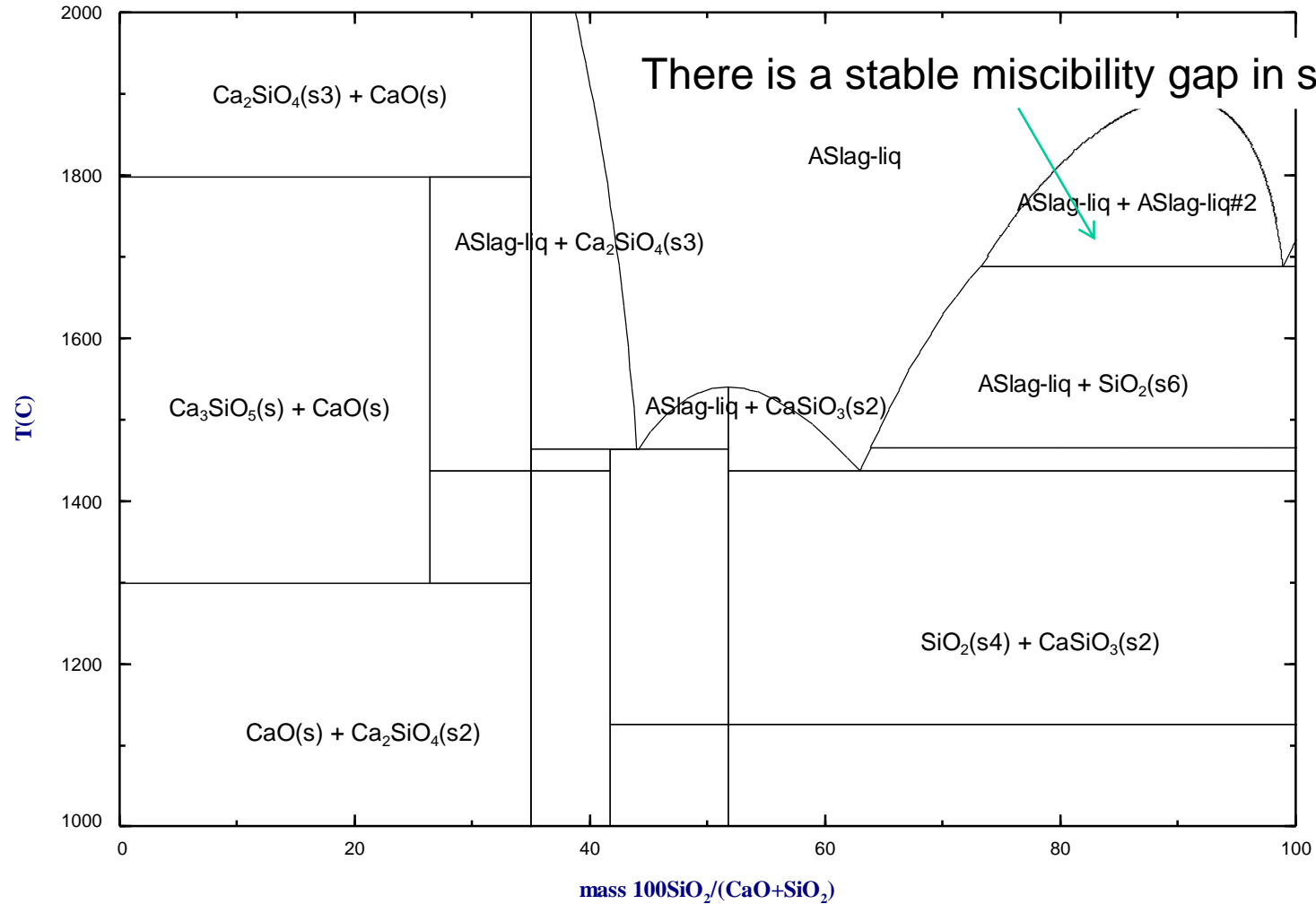
X

- no time limit - Calculate >>

FactSage 8.0

Binary phase diagram: CaO-SiO₂

CaO - SiO₂



Ternary phase diagram: CaO-SiO₂-Al₂O₃ isothermal section

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) CaO + SiO₂ + Al₂O₃

Products

Compound species

gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 30

species: 30

Target
 - none -
 Estimate T(K): 1000

Solution phases

□	+	Base-Phase	Full Name
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGA	A-Slag-liq all oxides + S
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-MeO_A	A-Monoxide
<input type="checkbox"/>	<input checked="" type="checkbox"/>	FToxid-Mel_A	A-Melilite
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-Mull	Mullite

Legend
 I - immiscible 3
 + - selected 1

species: 20
 solutions: 7

Variables

T(C)	SiO ₂ /CaO	Al ₂ O ₃ /CaO
1550	0.1	0.1

A = SiO₂, B = CaO, C = Al₂O₃

Phase Diagram

SiO₂
 CaO Al₂O₃
 - no time limit -

Variables: CaO-SiO₂-Al₂O₃ composition #1. vs composition #1.

Variables

compositions: 2
 log10(a): 0
 X,Y steps: 11

T and P

Temperature: constant
 1550

Pressure or Volume:
 P(atm): constant
 log P
 V(litre): 1
 log V

Compositions Quantity(g)

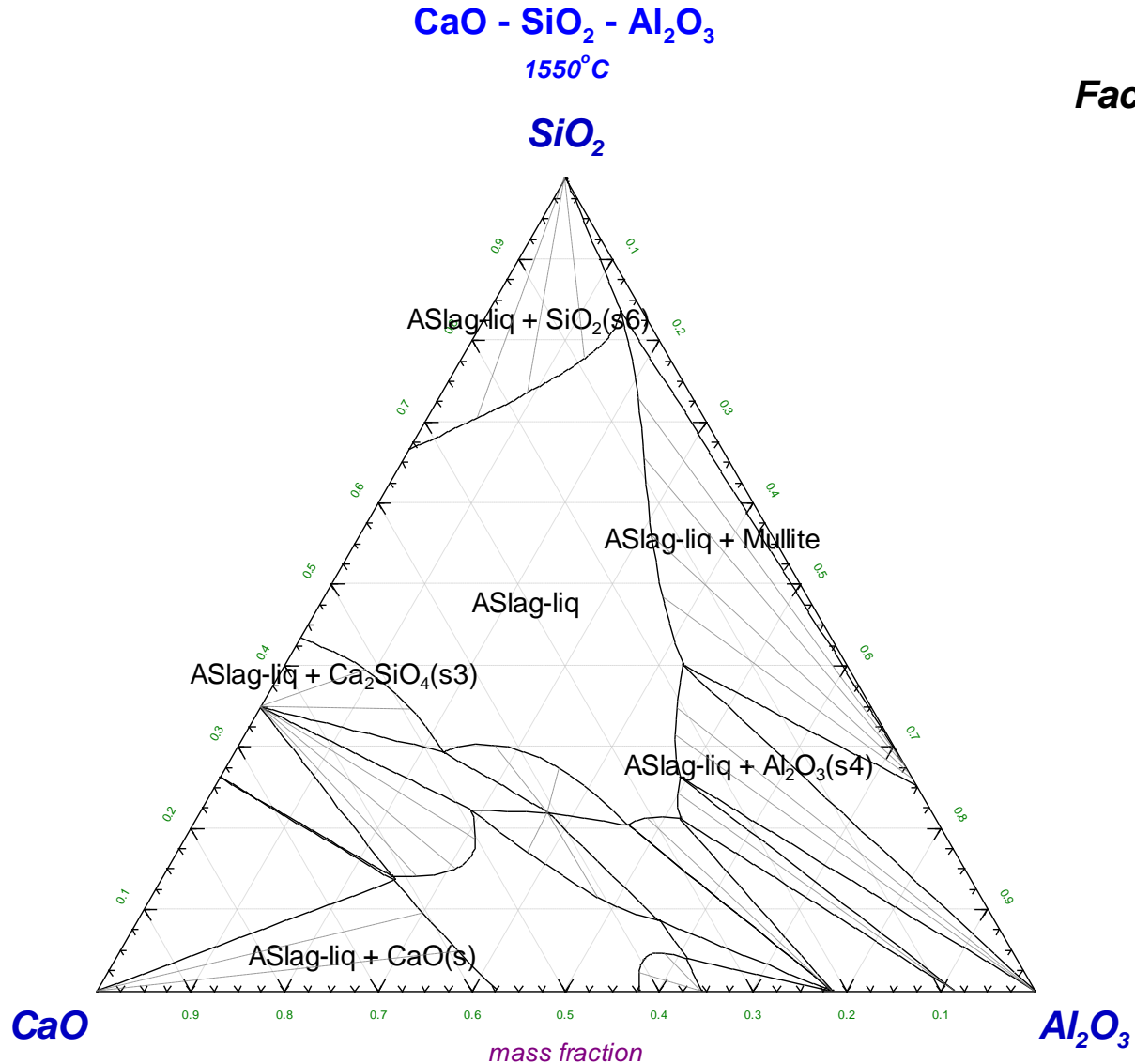
#1. 0 CaO + 1 SiO₂ + 0 Al₂O₃ = A-Corner
 1 CaO + 1 SiO₂ + 1 Al₂O₃ = 1 (max)
 0 (min)

#2. 0 CaO + 0 SiO₂ + 1 Al₂O₃ = C-Corner
 1 CaO + 1 SiO₂ + 1 Al₂O₃ = 1 (max)
 0 (min)

#3. 1 CaO + 0 SiO₂ + 0 Al₂O₃ = B-Corner
 1 CaO + 1 SiO₂ + 1 Al₂O₃ = 1 (max)
 0 (min)

Cancel OK

Ternary phase diagram: CaO-SiO₂-Al₂O₃ isothermal section



Ternary system: section in ternary (isopleth)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) CaO + SiO2 + Al2O3

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 30

species: 30

Target

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
I		FToxid-SLAGA	A-Slag-liq all oxides + S
I		FToxid-MeO_A	A-Monoxide
+		FToxid-Mel_A	A-Mellite
I		FToxid-Mull	Mullite

Legend

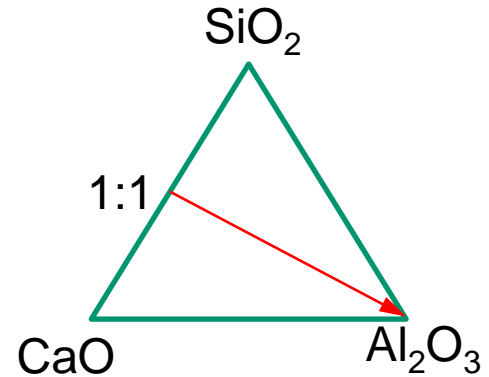
I - immiscible 3
+ - selected 1

Species: 20
Solutions: 7

Variables

T(C)	CaO-1SiO2/	100Al2O3/(CaO		
1000 1800	0 (min)	0 100		

T(C) vs 100Al2O3/(CaO+SiO2+Al2O3)



Variables: CaO-SiO2-Al2O3 T(C) vs composition #1.

Variables

Y-axis: T(C) 1/T(K)

X-axis: compositions 2 log10(a) 0

X,Y steps 11

Next >>

T and P

Temperature

Y-axis: T(C) 1/T(K)

Max: 1800
Min: 1000

Pressure or Volume

P(atm) constant log P V(litre) 1 log V

Compositions Quantity(g)

#1. $1 \text{ CaO} + -1 \text{ SiO}_2 + 0 \text{ Al}_2\text{O}_3 = \text{constant}$

#2. $0 \text{ CaO} + 0 \text{ SiO}_2 + 100 \text{ Al}_2\text{O}_3 = \text{X-axis}$

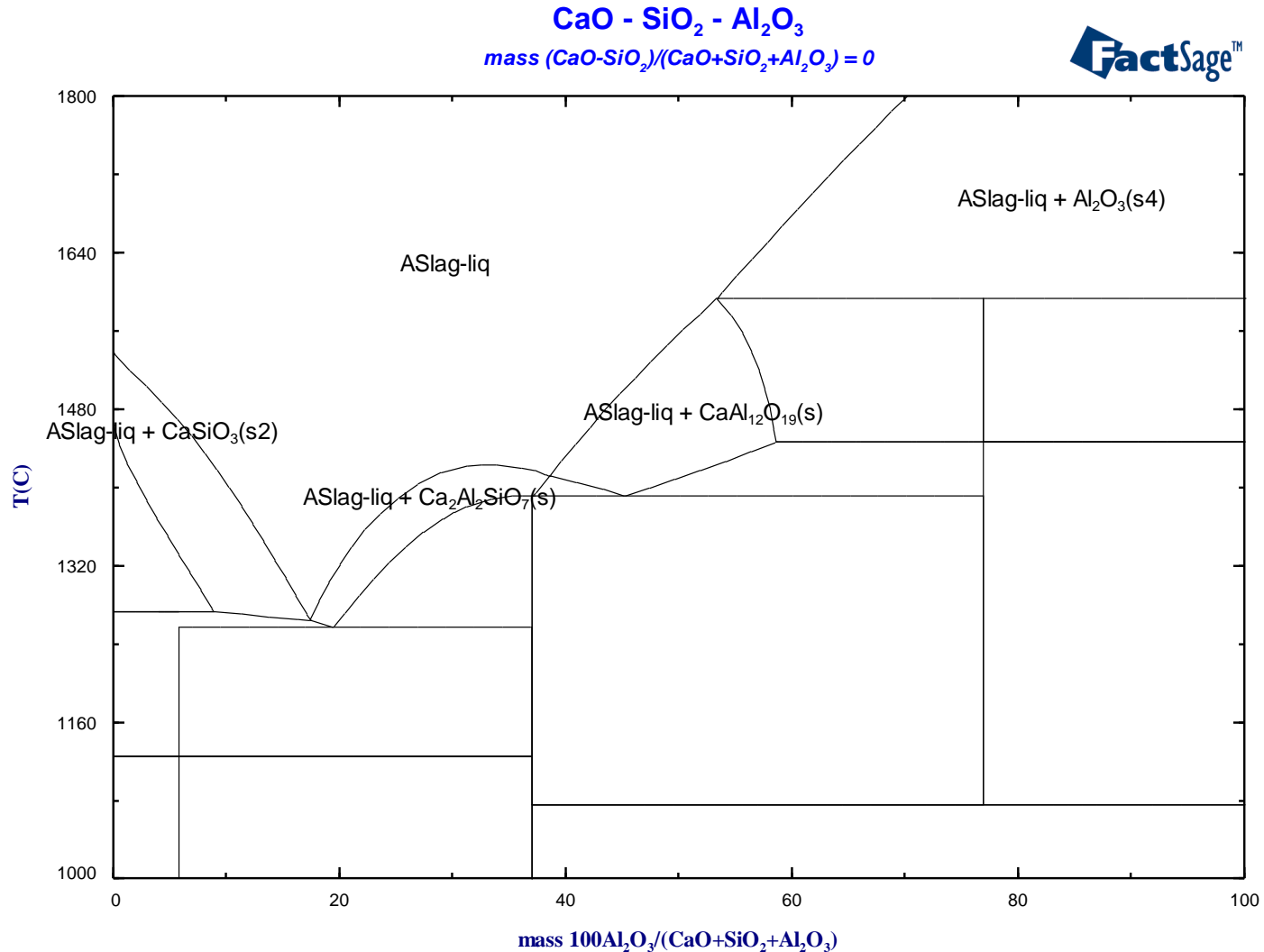
100 (max)
0 (min)

Cancel

OK

Ternary system: section in ternary (isopleth)

CaO-SiO₂-Al₂O₃ Vertical section at
(wt%CaO/wt%SiO₂) = 1



Oxidation diagram: Fe-Cr-O2

Data Search

Databases - 3/26 compound databases, 2/26 solution databases

Fact **FactSage** **SGTE**

FactPS FSopp BINS EXAM SGTEa SGTEb

FToxid FSlead SGPS SGTE

FTsalt FSstel SGTE

FTmisc FSupsi SGsold

FTall

FToxCN

FTfritz

FTthelg ELEM SGnobl

FTpulp FTdemo SpMCCBN

FTlite FTnucl TDmeph

TDnucl

compounds only
solutions only
no database

Clear All

Add/Remove Data

RefreshDatabases

Information

Options - search for product species

Default

Include compounds

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2

Cancel Summary ... OK

Combination of many databases:
 FACT53: gases (if necessary)
 FToxid: oxide phases
 FSstel: fcc, bcc and other metallic phases

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components {3}

Fe + Cr + O2

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 17

* - custom selection species: 17

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	+	FSstel-SIGM	SIGMA
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
	+	FToxid-CORU	M2O3(Corundum)

Legend

I - immiscible 3
 J - 3-immiscible 1
 + - selected 4

Show all selected

species: 52
 solutions: 13

Variables

T(C)	log10(p(O2))	(Fe+Cr)/(Fe+Cr)		
1600	-20.5	0.1		

log10 p(O2)/atm vs (Fe+Cr)/(Fe+Cr)

Custom Solutions

0 fixed activities
 0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 69
 Total Solutions (max 200) 13
 Total Phases (max 1500) 30

Phase Diagram

Y
 - no time limit -

FactSage 8.0

Oxidation diagram: Fe-Cr-O₂

Variables: Fe-Cr-O₂ log₁₀ p(O₂)/atm vs composition #1.

Variables

compositions 1

log₁₀(a) 1

T and P

Temperature

T(C) constant 1600

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Chemical Potentials

#1 log₁₀(p/atm) Y-axis

O₂ -5

gas-FactPS -20

Compositions Quantity(mol)

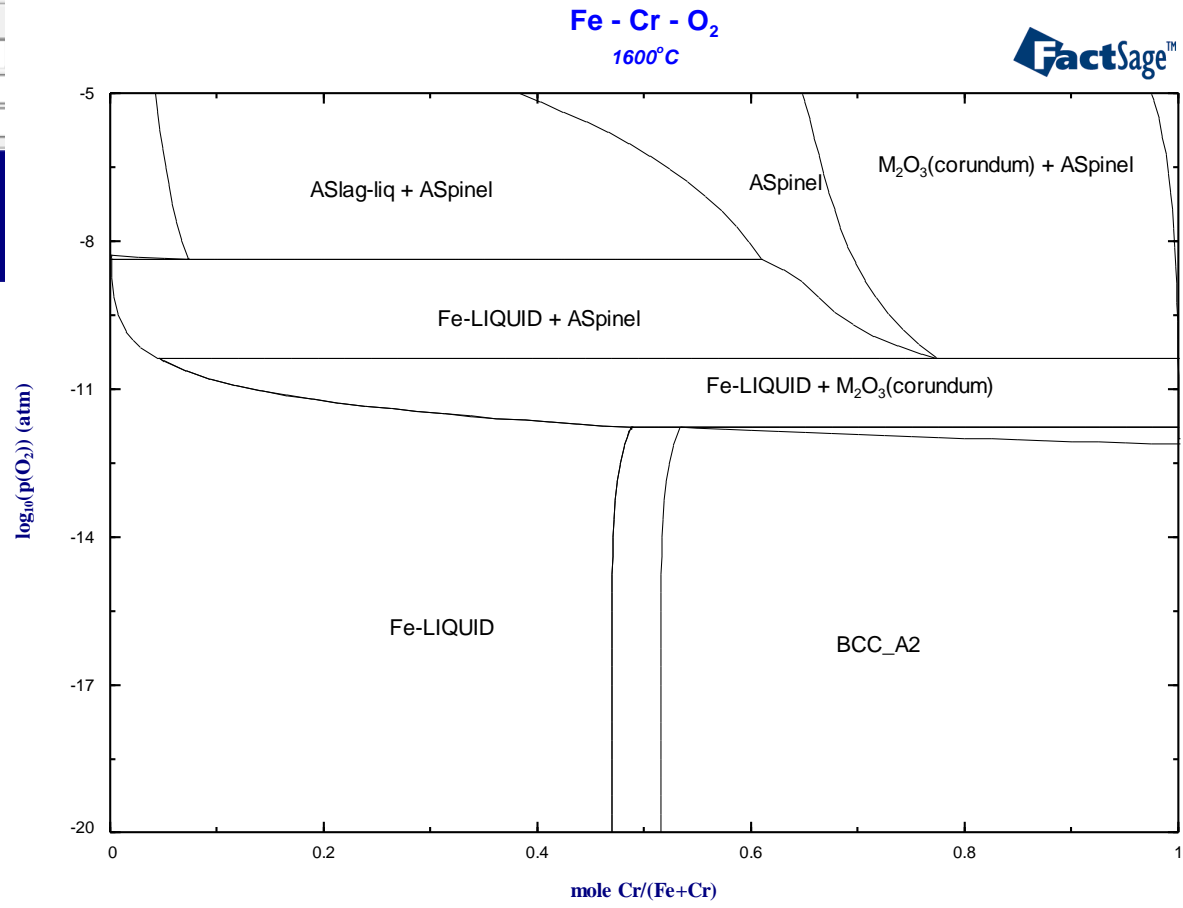
#1. 0 Fe + 1 Cr = 1 (max)

1 Fe + 1 Cr = 0 (min)

#1 log₁₀(composition)

Cancel

Log pO₂ for y-axis variable



Predominance diagram: Fe-Mn-O2-S2

Combination of many databases:
FACT53: gases (if necessary)
FToxid: oxide phases
FSStel: fcc, bcc and other metallic phases

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (4)

(gram) O2 + S2 + Fe + Mn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 30
- * - custom selection species: 30

Solution phases

*	+	Base-Phase	Full Name
I		FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
I		FSstel-HCP	HCP_A3
+		FSstel-CBCC	CBCC_A12
+		FSstel-CUB	CUB_A13
+		FSstel-MONO	Monoxide
+		FSstel-PYRR	Pyrrhotite

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit...

Volume data

- assume molar volumes of solids and liquids = 0
- include molar volume data and physical properties data

Target

Estimate T(K): 1000

Variables

T(C)	log10(p(O2))	log10(p(S2))	Mn/(Fe+Mn)
1300	-20.0	-20.0	0.3

log10 p(O2)/atm vs log10 p(S2)/atm

Variables: O2-S2-Fe-Mn log10 p(O2)/atm vs log10 p(S2)/atm

Variables

compositions 1

log10(a) 2

T and P

Temperature: T(C) constant 1300

Pressure or Volume: P(atm) constant 1

Chemical Potentials

#1 log10(p/atm) Y-axis

O2 0

gas-FactPS -20

#2 log10(p/atm) X-axis

S2 0

gas-FactPS -20

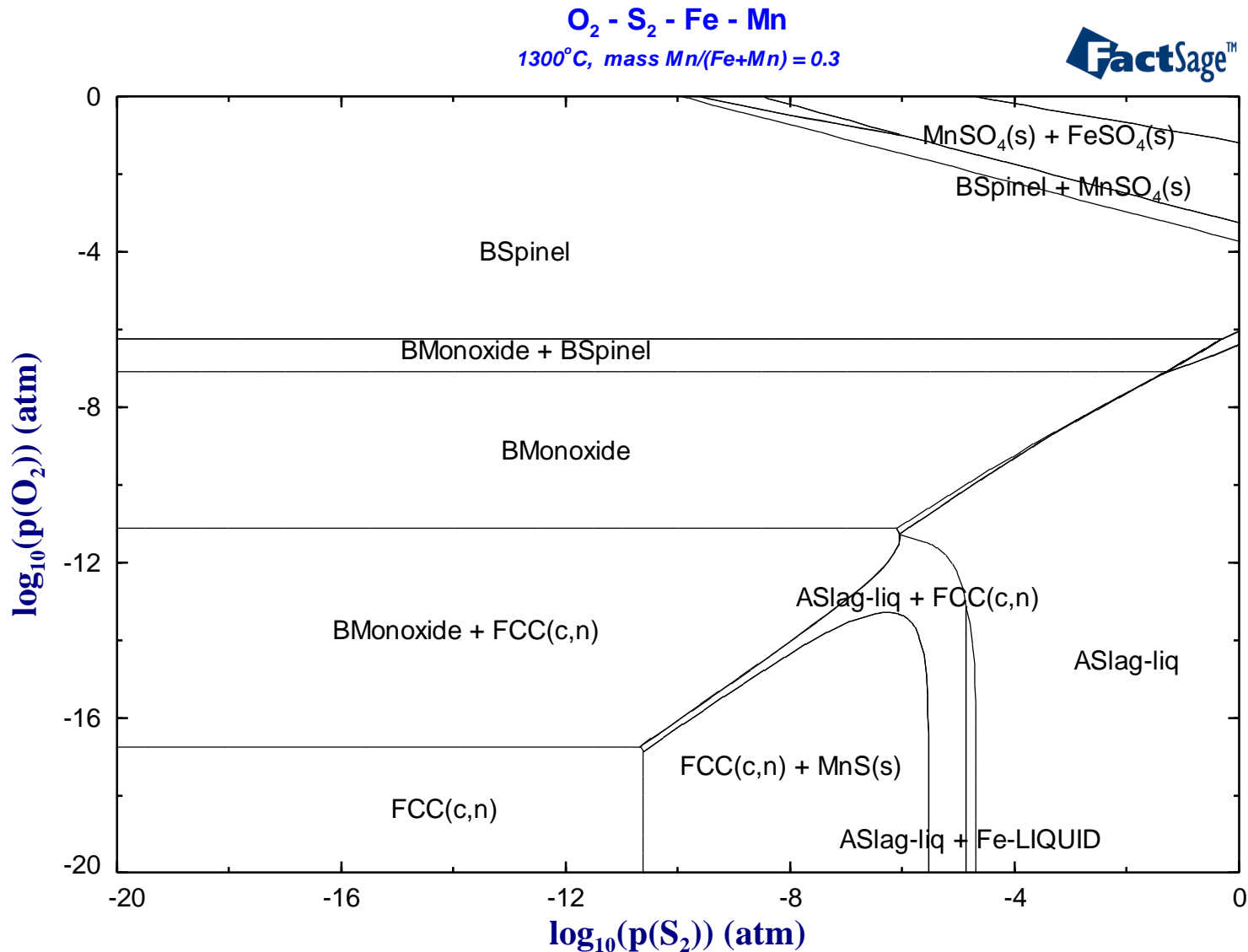
Compositions Quantity(g)

#1. 0 Fe + 1 Mn = constant

1 Fe + 1 Mn = 0.3

Cancel OK

Predominance diagram: Fe-Mn-O2-S2



Quaternary diagram: iso-composition section

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (4)

(gram) MgO + CaO + SiO2 + Al2O3

Products

Compound species

gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 50
 species: 50

Solution phases

+	Base-Phase	Full Name
+	FToxid-SLAGA	A-Slag-liq all oxides + S
+	FToxid-SPINA	A-Spinel
+	FToxid-MeO_A	A-Monoxide
+	FToxid-cPyrA	A-Clinopyroxene
+	FToxid-oPyrA	A-Orthopyroxene
+	FToxid-pPyrA	A-Protopyroxene
+	FToxid-LcPy	LowClinopyroxene
+	FToxid-WOLLA	A-Wollastonite

Custom Solutions
 0 fixed activities Details ...
 0 ideal solutions

Pseudonyms
 apply Edit ...

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 12
 Total Species (max 5000): 132

Legend
 - none
 Estimate T(K): 1000
 Show all selected
 - immiscible 5
 + selected 9

Variables

T(C)	MgO/(MgO)	CaO/(MgO+CaO)	Al2O3/(MgO)
1600	0.1	0.1	0.1 (min)

A = MgO, B = SiO2, C = CaO

FactSage 8.0

Variables: MgO-CaO-SiO2-Al2O3 composition #1. vs composition #1.

Variables

compositions: 3

log10(a): 0

X,Y steps: 11

T and P

Temperature: constant 1600

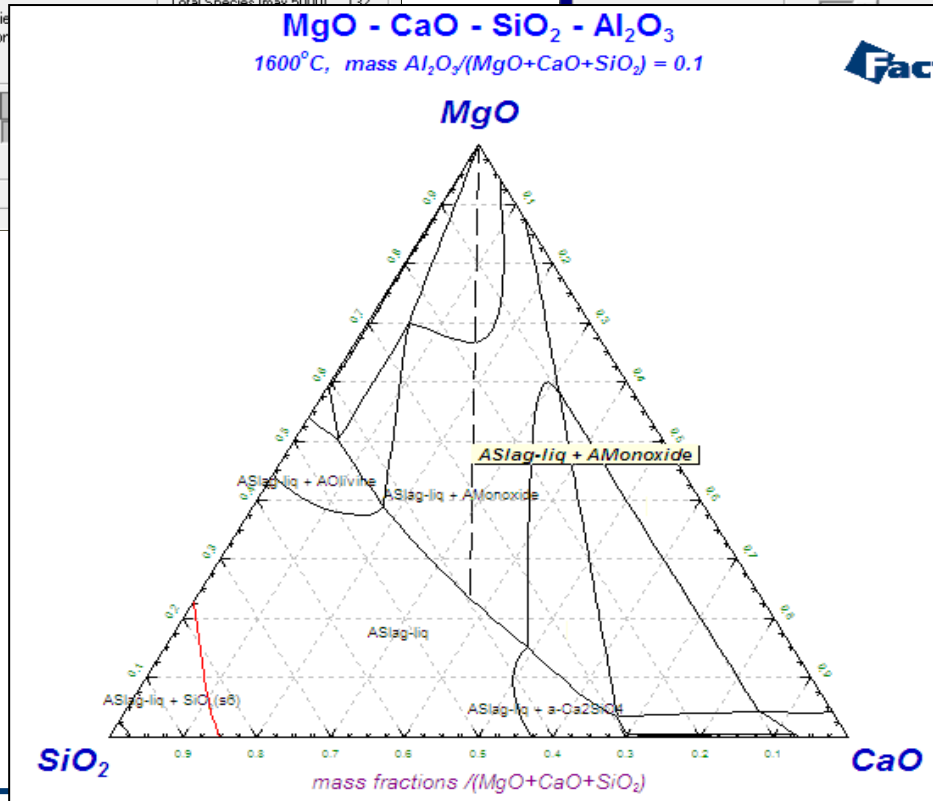
Pressure or Volume: constant 1

Compositions Quantity(g)

#1. 1 MgO + 0 CaO + 0 SiO2 + 0 Al2O3 = 1 (max)
 1 MgO + 1 CaO + 1 SiO2 + 0 Al2O3 = 0 (min)

Composition #

OK



Quaternary system: CaO-Ca₂SiO₄-MgAl₂O₄

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) MgAl₂O₄ + CaO + Ca₂SiO₄

Products

Compound species

gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 50
 species: 50

Target

none
 Estimate T(K): 1000

Variables

T(C)	L/(L+CaO+M)	CaO/(L+CaO+M)
1600	0.1	0.1

A = L, B = M, C = CaO - L=MgAl₂O₄ M=Ca₂SiO₄

FactSage 8.0

Variables: MgAl₂O₄-CaO-Ca₂SiO₄ composition #1. vs composition #1.

Variables

compositions 2

log10(a) 0

X,Y steps 11

T and P

Temperature

T(C) constant 1600

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Compositions Quantity(g)

L=MgAl₂O₄ M=Ca₂SiO₄

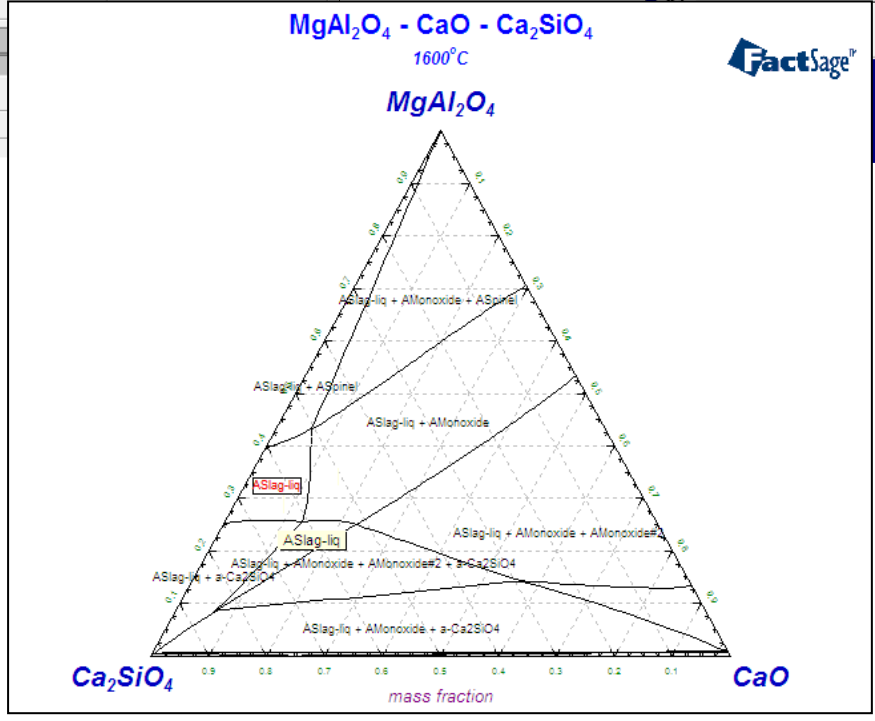
#1. 1 L + 0 CaO + 0 M = 1 (max) 0 (min)

#2. 0 L + 1 CaO + 0 M = 1 (max) 0 (min)

0 L + 0 CaO + 1 M = 1 (max) 0 (min)

0 L + 1 CaO + 1 M = 1 (max) 0 (min)

Cancel OK



Fe oxide containing system: Fe saturation

Intentional addition of Fe to make Fe saturation

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 1/6 LIQUID Duplicates selected X denotes species excluded by default

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	11	Si(liq)	FactPS	liquid		V			
X	12	SiO2(liq)	FactPS	liquid		V			
+	13	Fe(liq)	FactPS	liquid		V			
	14	FeO(liq)	FactPS	liquid		V			
X	15	Fe3O4(liq)	FactPS	liquid		V			
	16	SiO2(liq)	FToxid	liquid		V			

permit selection of 'X' species Help Suppress Duplicates Edit priority list:

Show Selected Select All Select/Clear... Clear OK

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components [3]

(gram) FeO + SiO2 + Fe

Products

Compound species

gas ideal real 0
 aqueous 0
 pure liquids 1
 pure solids 24
 * - custom selection species: 25

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
	+	FToxid-cPyrA	A-Clinopyroxene

Legend

I - immiscible 1
+ - selected 3

Show all selected

species: 18 Select
solutions: 5

Custom Solutions

fixed activities Details ...
 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 6
Total Species (max 5000) 43
Total Solutions (max 200) 5
Total Phases (max 1500) 30

Variables

T(C)	SiO2/(FeO+SiO2)	Fe/(FeO+SiO2)		
500 2000	0 1	0.001		

T(C) vs SiO2/(FeO+SiO2)

Phase Diagram

Y X

- no time limit - Calculate >>

- recommend you not select both pure liquids and molten solutions -

FactSage 8.0

Fe oxide containing system: Fe saturation

Variables: FeO-SiO2-Fe T(C) vs composition #1.

Variables

compositions: 2

log10(a): 0

T and P

Temperature: T(C) (Y-axis)

Max: 2000, Min: 500

Pressure or Volume: P(atm) constant, V(litre) 1, log V

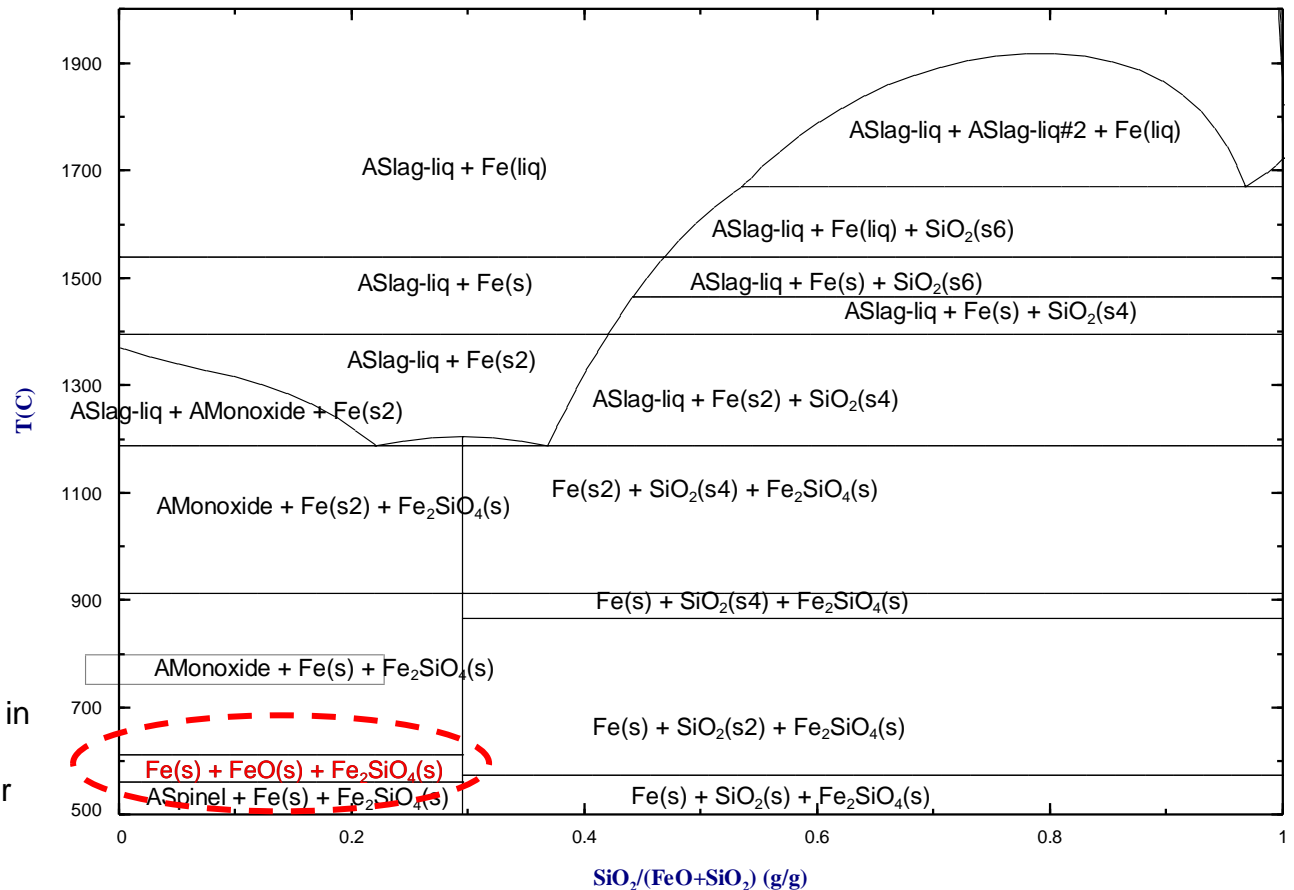
Compositions Quantity(g)

#1: 0 FeO + 1 SiO2 + 0 Fe = 1 (max) / 0 (min)

#2: 0 FeO + 0 SiO2 + 1 Fe = constant / 0.001

Cancel

FeO - SiO₂ - Fe
 $Fe/(FeO+SiO_2) \text{ (g/g)} = 0.001$



Intentional addition of Fe to make Fe saturation

Monoxide = FeO. But due to slightly different Gibbs energies of FeO stored in two databases, FeO from FACT53 appears in the calculation. → for better calcs, remove FeO(s) from database selection

Fe oxide containing system: fixed PO₂

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) FeO + SiO₂ + O₂

Products

Compound species

- gas ideal real 0
- aqueous 0
- + pure liquids 1
- + pure solids 24
- * - custom selection species: 25

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
	+	FToxid-cPyrA	A-Clinopyroxene

Custom Solutions:

- 0 fixed activities
- 0 ideal solutions

Pseudonyms: apply Edit ...

Volume data:

- assume molar volumes of solids and liquids = 0
- include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 6

Total Species (max 5000) 43

Total Solutions (max 2000) 5

Total Phases (max 150)

Target: none - Estimate T(K): 1000

Legend: I - immiscible 1, +- selected 3

Show all selected

species: 18 Select

solutions: 5

Variables

T(C)	log ₁₀ (p(O ₂))	SiO ₂ /(FeO+SiO ₂)
500 2000	-10	0 1

T(C) vs SiO₂/(FeO+SiO₂)

Phase Diagram

Y X

- no time limit - Calculate

- recommend you not select both pure liquids and molten S

FactSage 8.0

Fixing PO₂ to control the oxidation state of Fe

Variables: FeO-SiO₂-O₂ T(C) vs composition #1.

Variables

compositions 1

log₁₀(a) 1

Next >>

T and P

Temperature

- T(C) Y-axis
- 1/TK

Max: 2000

Min: 500

Pressure or Volume

- P(atm) constant
- log P
- V(litre) 1
- log V

Chemical Potentials

#1 log₁₀(p/atm) constant

O₂

gas-FactPS -10

Compositions Quantity(g)

#1. 0 FeO + 1 SiO₂ = X-axis

1 FeO + 1 SiO₂ = 1 (max)

0 (min)

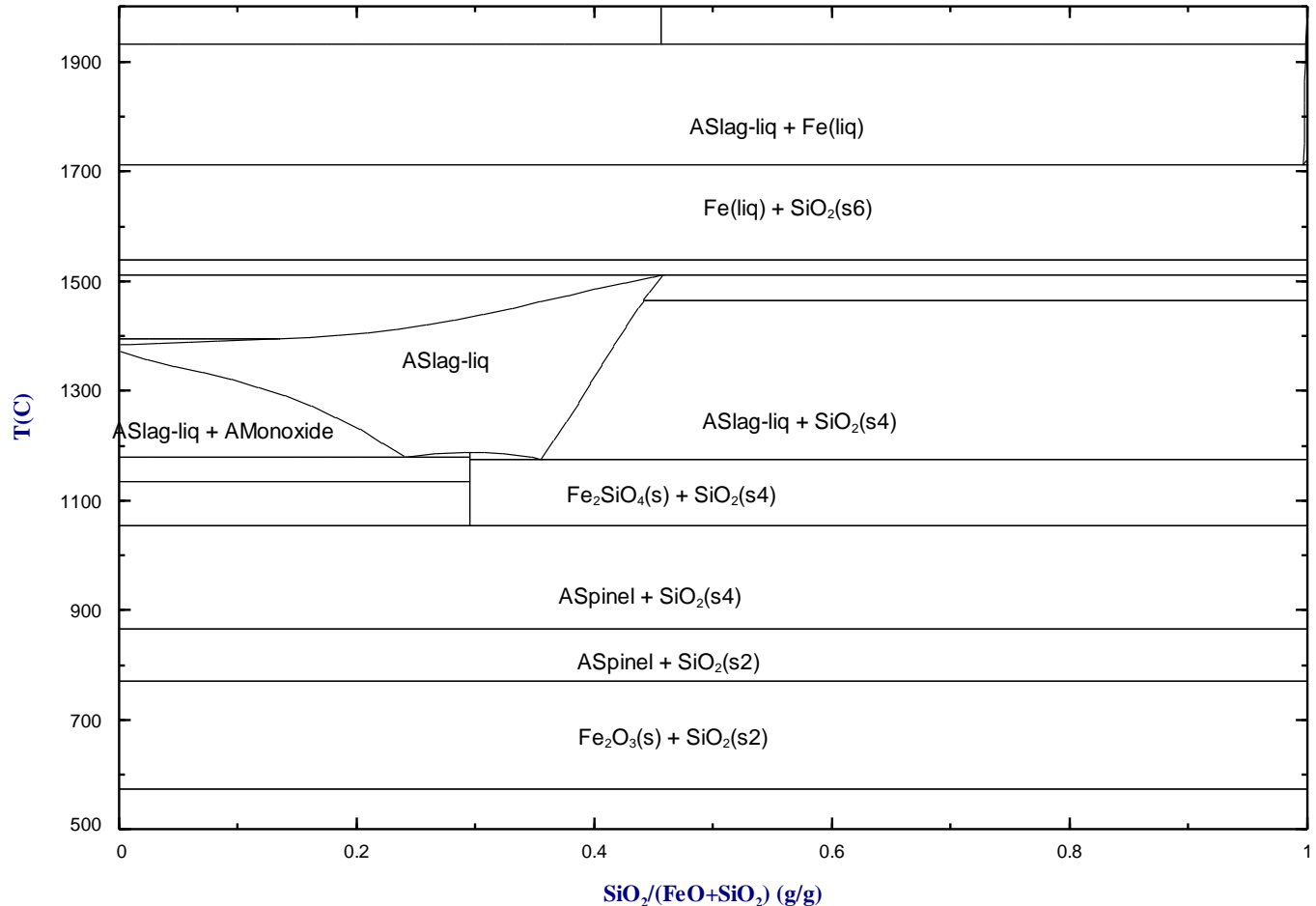
#1 log₁₀(composition)

Cancel OK

Fe oxide containing system: fixed PO₂

When PO₂ is fixed with selection of Fe, slag and Fe oxides can be reduced by Oxygen to Fe at certain temperature and composition

FeO - SiO₂ - O₂
 $p(O_2) = 10^{-10}$ atm



Fe oxide containing system: fixed CO/CO2 gas

Fixing PO_2 by CO/CO2 gas mixture

Selection - Phase Diagram - no results -

Selected: 3/23 **GAS** X denotes species excluded by default

- no results -

+ Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	C(g)	FactPS	gas					
2	C2(g)	FactPS	gas					
3	C3(g)	FactPS	gas					
4	C4(g)	FactPS	gas					
5	C5(g)	FactPS	gas					
6	O(g)	FactPS	gas					
7	O2(g)	FactPS	gas					
8	O3(g)	FactPS	gas					
9	CO(g)	FactPS	gas					
10	C2O(g)	FactPS	gas					
11	CO2(g)	FactPS	gas					
12	C3O2(g)	FactPS	gas					
13	Si(g)	FactPS	gas					
14	Si2(g)	FactPS	gas					
15	Si3(g)	FactPS	gas					
16	SiC(g)	FactPS	gas					
17	SiC2(g)	FactPS	gas					
18	Si2C(g)	FactPS	gas					
19	SiO(g)	FactPS	gas					
20	SiO2(g)	FactPS	gas					
21	Fe(g)	FactPS	gas					

permit selection of 'X' species Help Suppress Duplicates Edit priority list

Show Selected Select All Select/Clear... Clear OK

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (4)

FeO + SiO2 + CO + CO2

Products

Compound species

- gas ideal real 3
- aqueous 0
- pure liquids 1
- pure solids 31
- * - custom selection species: 35

Target: none - Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SLAG?	?-Slag-liq
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
	+	FToxid-cPyrA	A-Clinopyroxene

Legend: I - immiscible 1, + - selected 3

Show all selected

species: 18 solutions: 5 Select

Variables

T(C)	SiO2/(FeO+SiO2)	CO/(FeO+SiO2)	CO2/(FeO+SiO2)
500 2000	0.1	0.9 (min)	0.1 (min)

T(C) vs SiO2/(FeO+SiO2)

Phase Diagram: Y vs X, - no time limit - Calculate >>

Virtual species: 6
 Total Species (max 5000): 53
 Total Solutions (max 200): 5
 Total Phases (max 1500): 38

recommnd you not select both pure liquids and molten solutions -

FactSage 8.0

Select only CO, CO2 and O2 gas to simulate real experiment of oxide/gas equilibration.
 → If we select all gases, some amount of oxides can be evaporated depending on the relative amount of gas and oxide in the calculations

Fe oxide containing system: fixed CO/CO2 gas

Variables: FeO-SiO2-CO-CO2 T(C) vs composition #1

Variables

compositions: 3

log10(a): 0

T and P

Temperature: Y-axis

T(C) Max: 2000 Min: 500

1/TK

Pressure or Volume: constant

P(atm) log P V(litre) 1 log V

Compositions Quantity(mol)

#1. 0 FeO + 1 SiO2 + 0 CO + 0 CO2 = 1 (max)

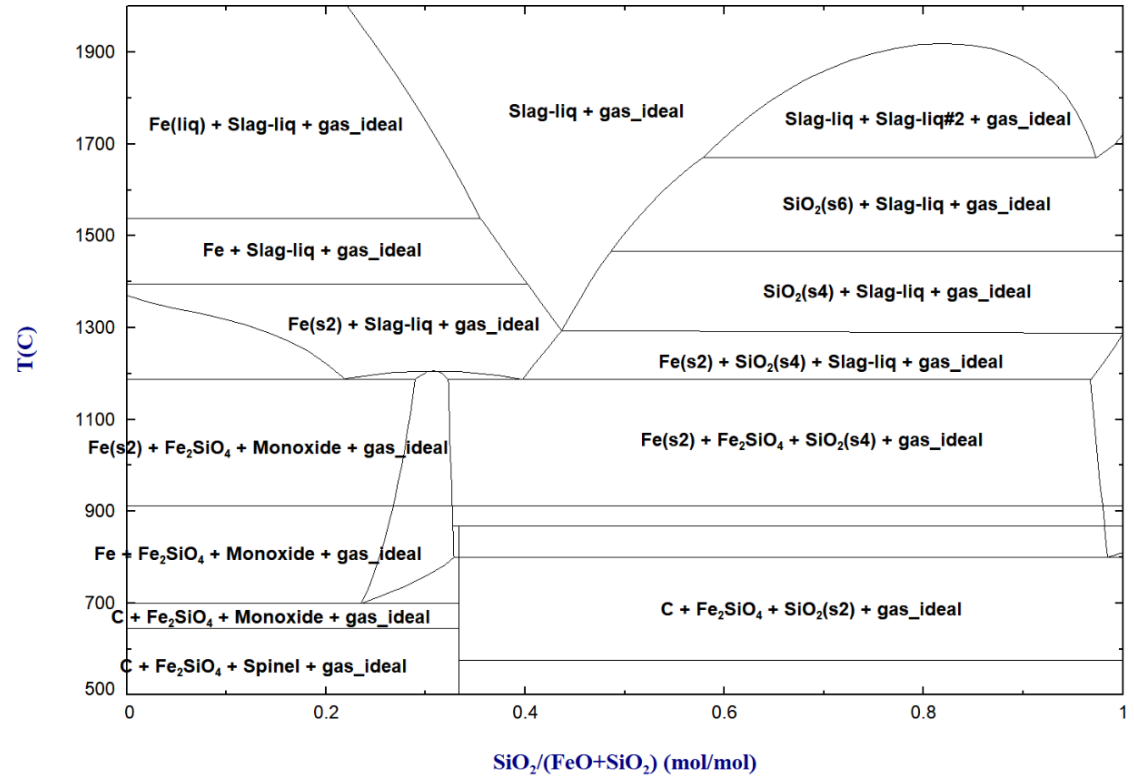
#2. 0 FeO + 0 SiO2 + 1 CO + 0 CO2 = constant

#3. 0 FeO + 0 SiO2 + 0 CO + 1 CO2 = constant

Cancel

Fixing CO/CO2 ratio

FeO - SiO₂ - CO - CO₂
 CO/(FeO+SiO₂)(mol/mol)=0.9, CO₂/(FeO+SiO₂)(mol/mol)=0.1,
 1 atm



Fe oxide containing system: fixed CO/CO2 gas

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (3)

Fe2O3 + CO + CO2

Products

Compound species

- gas ideal real 15
- aqueous 0
- pure liquids 0
- pure solids 11
- custom selection species: 26

Target

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-Liqu	LIQUID
	J	FSstel-FCC	FCC_A1
	I	FSstel-BCC	BCC_A2
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide

Legend

- I - immiscible 3
- J - 3-immiscible 1
- + - selected 2

Virtual species: 8

Total Species (max 5000) 64

Total Solutions (max 200) 11

Total Phases (max 1500) 23

Variables

T(C)	CO/(CO+CO2)	Fe2O3/(CO+CO2)
0 2000	0 1	0.1 (min)

T(C) vs CO/(CO+CO2)

Phase Diagram

Calculate >>

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 15/17

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	1	O(g)	FactPS	gas					
+	2	C2(g)	FactPS	gas					
+	3	C3(g)	FactPS	gas					
+	4	C4(g)	FactPS	gas					
+	5	C5(g)	FactPS	gas					
+	6	O(g)	FactPS	gas					
+	7	O2(g)	FactPS	gas					
+	8	O3(g)	FactPS	gas					
+	9	CO(g)	FactPS	gas					
+	10	C2O(g)	FactPS	gas					
+	11	CO2(g)	FactPS	gas					
+	12	C3O2(g)	FactPS	gas					
+	13	Fe(g)	FactPS	gas					
+	14	FeO(g)	FactPS	gas					
+	15	Fe(CO)5(g)	FactPS	gas					
X	16	O2(g)	FSstel	gas					
X	17	FeO(g)	FSstel	gas					

permitted selection of 'X' species

Show Selected Select All Select/Clear... Clear OK

Variables: Fe2O3-CO-CO2 T(C) vs composition #1.

Variables

compositions 2

log10(a) 0

Next >>

T and P

Temperature

T(C) Y-axis

Max: 2000

Min: 0

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Compositions Quantity(mol)

#1. 0 Fe2O3 + 1 CO + 0 CO2 = X-axis

0 Fe2O3 + 1 CO + 1 CO2 = 1 (max)

0 (min)

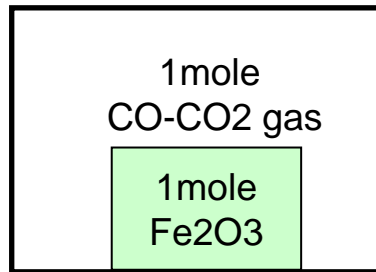
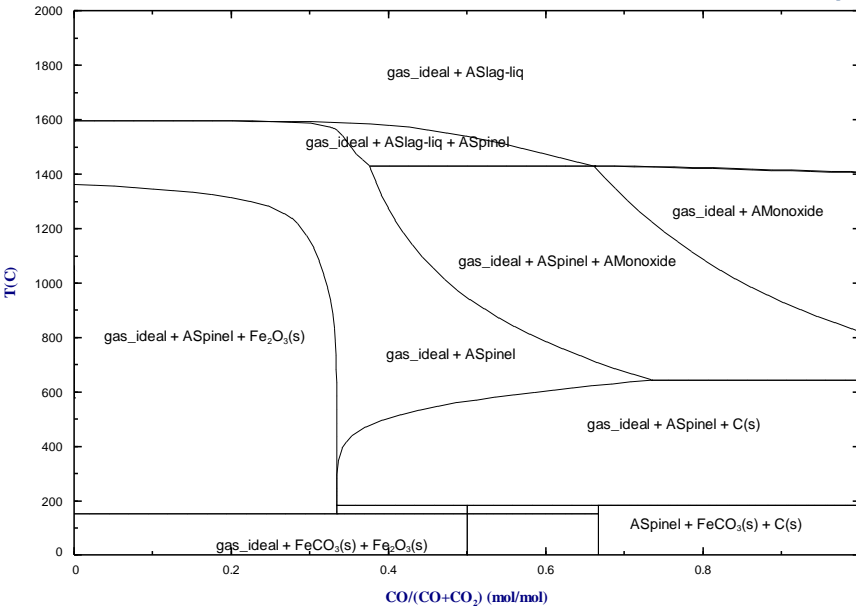
#2. 1 Fe2O3 + 0 CO + 0 CO2 = constant

0 Fe2O3 + 1 CO + 1 CO2 = 0.1

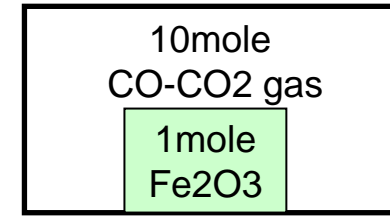
Cancel OK

Fe oxide containing system: fixed CO/CO₂ gas

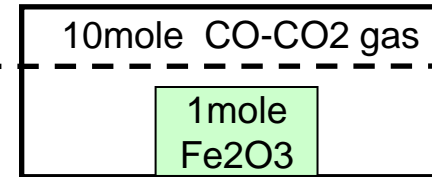
Fe₂O₃ - CO - CO₂
 $Fe_2O_3/(CO+CO_2) \text{ (mol/mol)} = 1$



<Closed system>

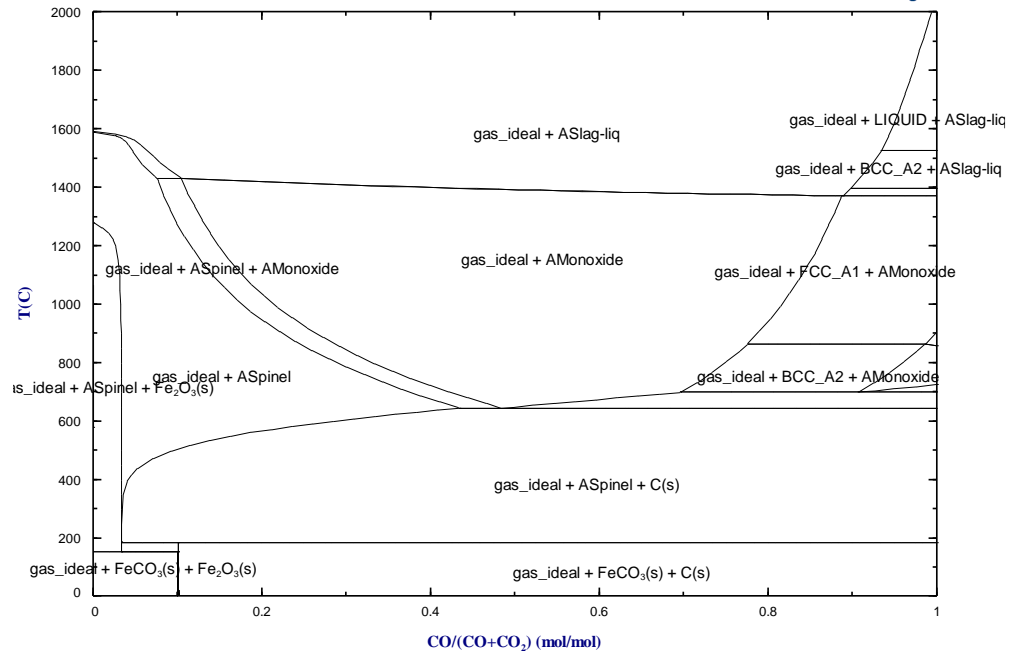


<Closed system>



<Open system>

Fe₂O₃ - CO - CO₂
 $Fe_2O_3/(CO+CO_2) \text{ (mol/mol)} = 0.1$



CaO-FeO-SiO₂ system with Fe saturation

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (4)

(gram) SiO₂ + FeO + CaO + Fe

Products

Compound species

gas ideal real 0

aqueous 0

* pure liquids 6

* pure solids 44

* custom selection species: 50

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	I	FToxid-MeO_A	A-Monoxide
	+	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,
	+	FToxid-bC2SA	A-a[Ca,Sr,Ba]2SiO4
	+	FToxid-aC2SA	A-a[Ca,Sr]2SiO4
	+	FToxid-MeL_A	A-Melilite

Legend

I - immiscible 3

+ - selected 6

species: 46

solutions: 12

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

Variables: SiO₂-FeO-CaO-Fe composition #1. vs composition #1.

Variables

compositions 3

log₁₀(a) 0

X,Y steps 11

T and P

Temperature

T(C) constant 1650

Pressure or Volume

P(atm) constant 1

log P

V(litre)

log V

Phase Diagram

siO₂

CaO

- no time li

Variables

T(C)	SiO ₂ /(SiO ₂ +FeO)	FeO/(SiO ₂ +FeO)	Fe/(SiO ₂ +FeO)
1650	0.1	0.1	0.001 (min)

A = SiO₂, B = CaO, C = FeO

- recommend you not select both pure liqu

Compositions Quantity(g)

0 SiO₂ + 0 FeO + 0 CaO + 1 Fe = Constant

#4. 1 SiO₂ + 1 FeO + 1 CaO + 0 Fe = 0.001

#4 log₁₀(composition)

Composition #

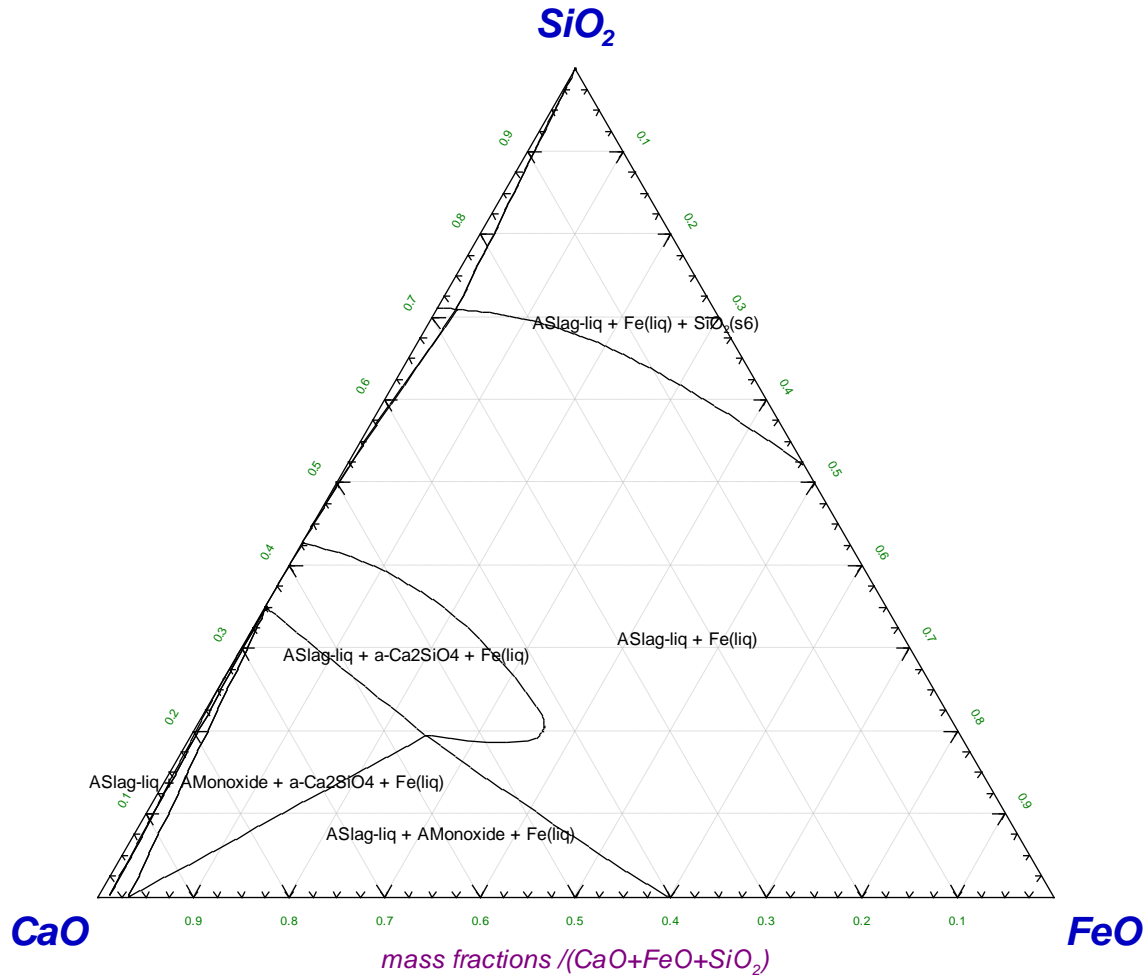
#4 max = 4

Cancel OK

FactSage 8.0

CaO-FeO-SiO₂ system with Fe saturation

CaO - FeO - SiO₂ - Fe
1650°C, Fe/(CaO+FeO+SiO₂) (g/g) = 0.001



CaO-FeO-SiO₂-5wt%MgO system with Fe saturation

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (5)

(gram) SiO₂ + FeO + CaO + MgO + Fe

Products

Compound species

gas ideal real 0

aqueous 0

* pure liquids 8

* pure solids 61

* - custom selection species: 69

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
	+	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite,

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volumes of solids and liquids

paraequilibrium

Virtual species

Total Species

Total Solution

Total Phases

Variables

compositions 4

log10(a) 0

X,Y steps 11

Next >>

T and P

Temperature

T(C) constant 1650

Pressure or Volume

P(atm) constant

log P

V(litre) 1

log V

Variables

T(C)	SiO ₂ /(SiO ₂ +FeO)	FeO/(SiO ₂ +FeO)	MgO/(SiO ₂ +FeO)	Fe/(SiO ₂ +FeO)
1650	0.1	0.1	0.05 (min)	0 (min)

A = SiO₂, B = CaO, C = FeO

Phase Diagram

SiO₂

CaO FeO

- no time limit -

- recommend you not select both pure liquids and pure solids

FactSage 8.0

Variables: SiO₂-FeO-CaO-MgO-Fe composition #1. vs composition #1.

Compositions Quantity(g)

#4. 0 SiO₂ + 0 FeO + 0 CaO + 1 MgO + 0 Fe = Constant

1 SiO₂ + 1 FeO + 1 CaO + 1 MgO + 1 Fe = 0.05

#4 log10(composition)

Composition #

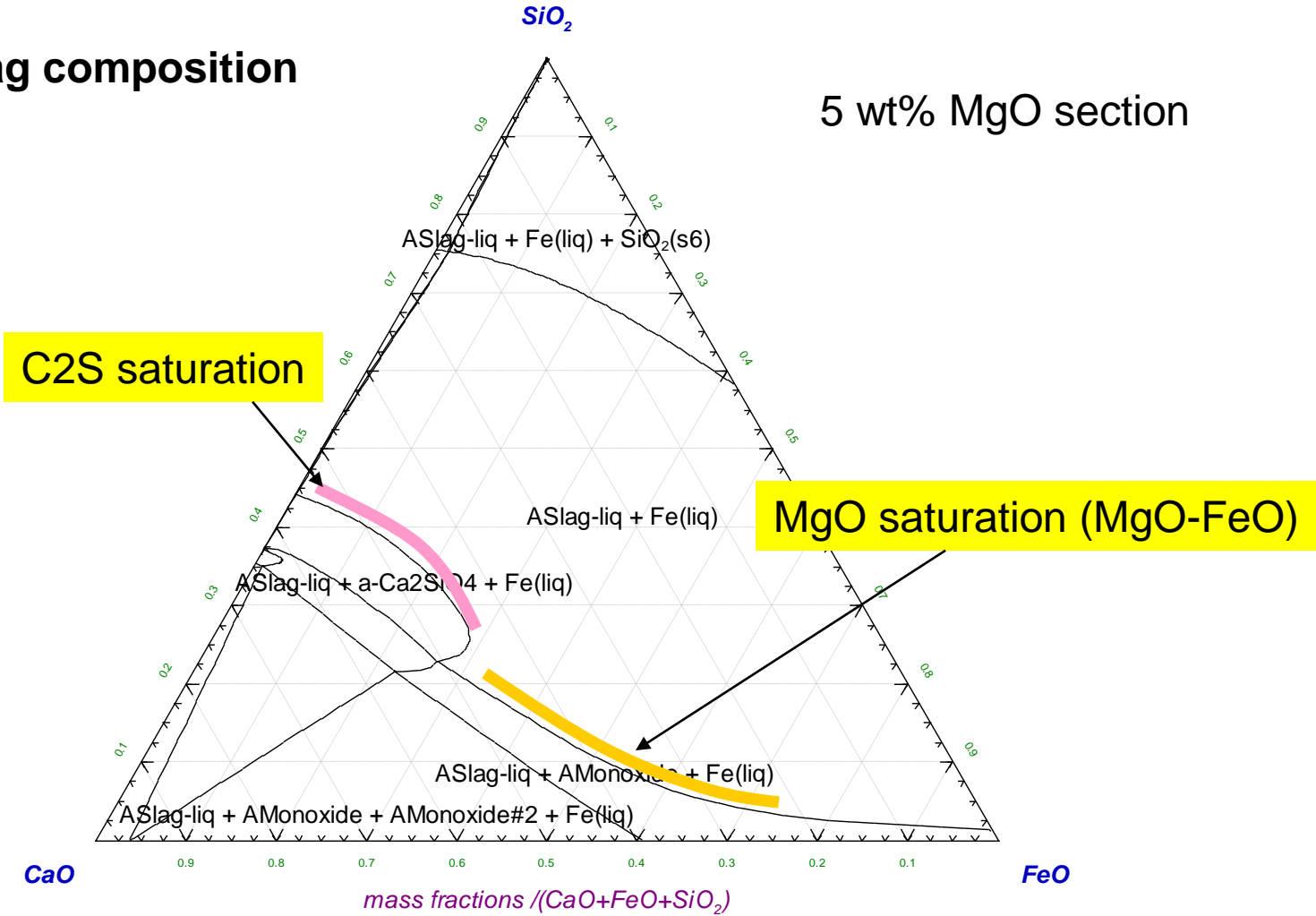
#4 max = 5

Cancel OK

CaO-FeO-SiO₂-5wt%MgO system with Fe saturation

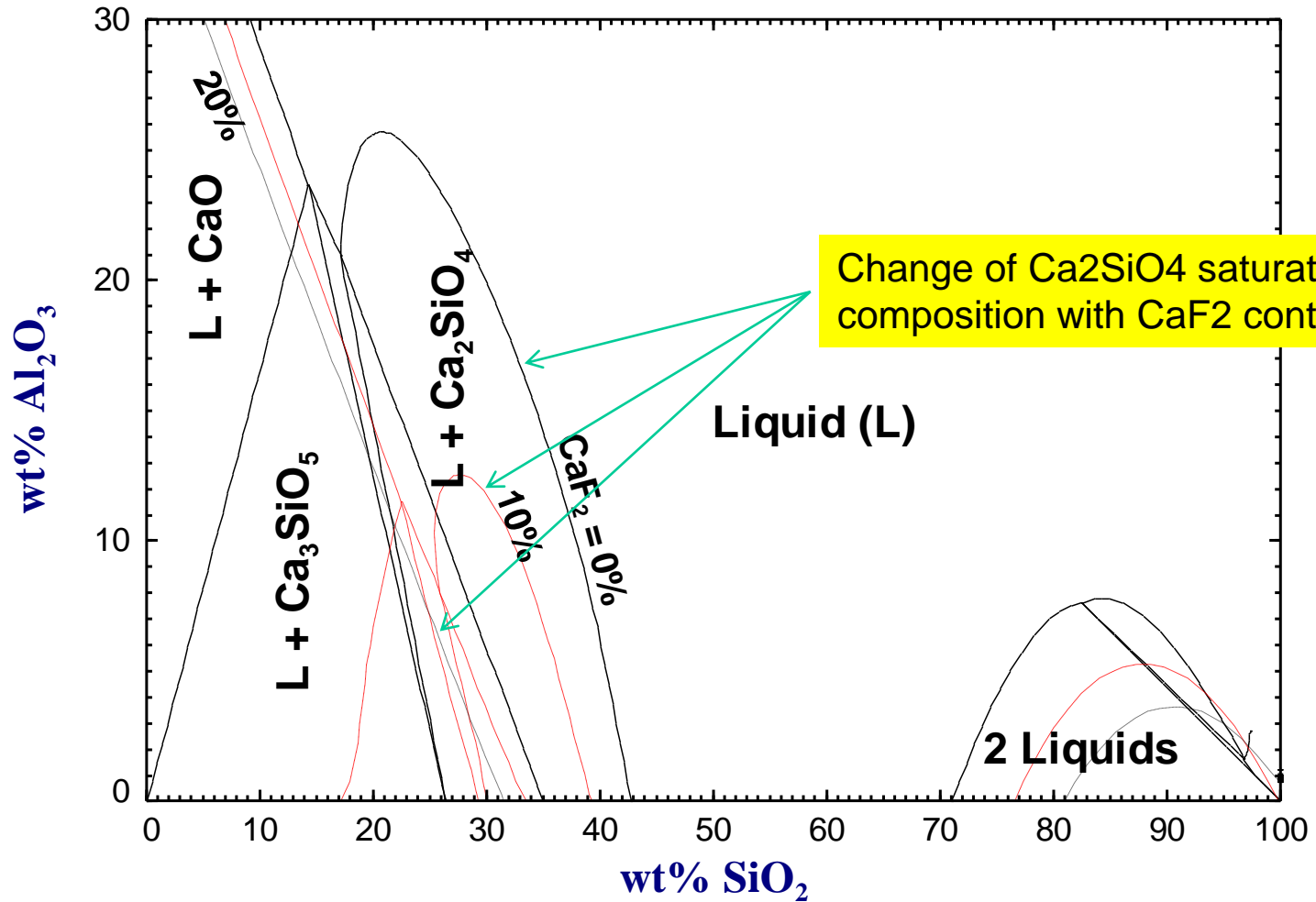
BOF slag composition

5 wt% MgO section



CaO-SiO₂-Al₂O₃ + F slags for refining flux

CaO-Al₂O₃-SiO₂ with various CaF₂ content at 1650°C.

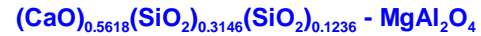


At 20% CaF₂: Slag can directly equilibrate with CaO (no Ca₂SiO₄)

CaO-Al₂O₃-SiO₂ slag – MgAl₂O₄ refractory

50%CaO-30%SiO₂-20%Al₂O₃ slag → in mole: (CaO)_{0.5618}(SiO₂)_{0.3146}(Al₂O₃)_{0.1236}
 (Equilib or Phase Diagram's components are in molar base)

Dissolution of spinel inclusion into slag



Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (2)

(gram) (CaO)0.5618(SiO2)0.3146(SiO2)0.1236 + MgAl2O4

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 50

species: 50

Target

none

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	I	FToxid-MeD_A	A-Monoxide
	I	FToxid-cPyrA	A-Clinopyroxene
	+	FToxid-oPyrA	A-Orthopyroxene
	+	FToxid-pPyrA	A-Protopyroxene
	+	FToxid-LcPy	LowClinopyroxene
	+	FToxid-WOLLA	A-Wollastonite

Legend

I - immiscible 5

+ - selected 9

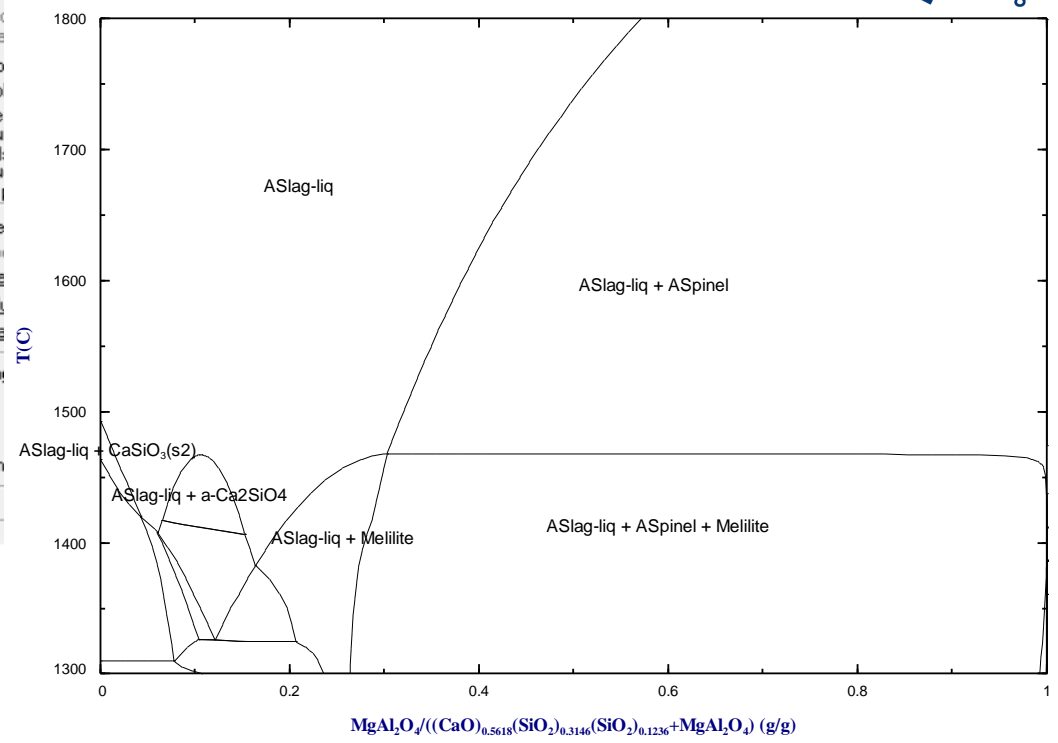
Show all selected

species: 82

solutions: 19

Phase Diagram

T(C) vs M/(L+M) - L=(CaO)0.5618(SiO2)0.3146(SiO2)0.1236 M=MgAl2O4



CaO-Al₂O₃-SiO₂ slag – MgAl₂O₄/Al₂O₃ refractories

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) (CaO)0.5618(SiO₂)0.3146(SiO₂)0.1236 + MgAl₂O₄ + Al₂O₃

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

pure solids 50

species: 50

Target

- none -

Estimate T(K): 1000

Variables

T(C)	L/(L+M+Al ₂ O ₃)	M/(L+M+Al ₂ O ₃)
1600	0.1	0.1

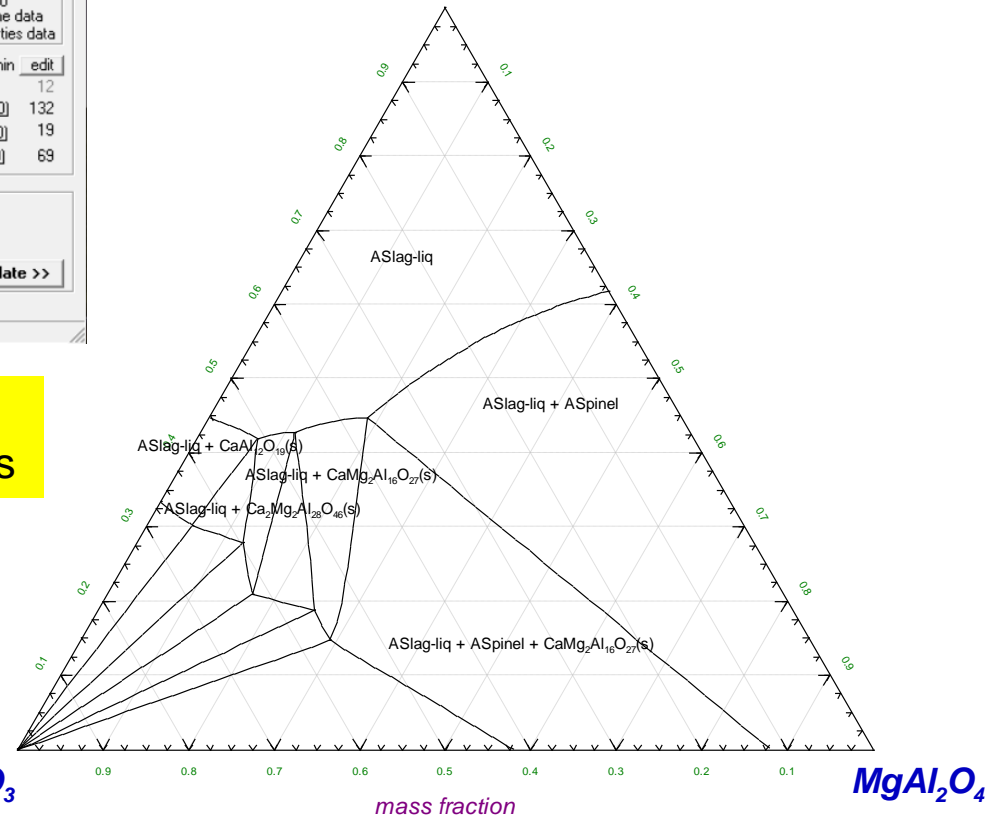
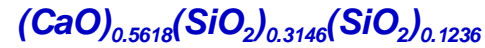
A = L, B = Al₂O₃, C = M · L=[CaO]0.5618[SiO₂]0.3146[SiO₂]0.1236 M=MgAl₂O₄

Phase Diagram

0.5618(SiO₂)0.3146(SiO₂)

Al₂O₃ MgAl₂O₄

- no time limit - Calculate >>



High Alumina (MgAl₂O₄-Al₂O₃)
Refractories dissolution into slags

CaO-Al₂O₂-SiO₂ slag – MgAl₂O₄/MgO refractories

Variables: (CaO)_{0.5618}(SiO₂)_{0.3146}(SiO₂)_{0.1236}-MgAl₂O₄-MgO composition #1. vs composition #1. X

Variables

Y-axis: X a b c d

log10(a):

T and P

Temperature: T(C)

Pressure or Volume: P(atm) log P V(litre) log V

Compositions Quantity(g)

L=(CaO)_{0.5618}(SiO₂)_{0.3146}(SiO₂)_{0.1236} M=MgAl₂O₄

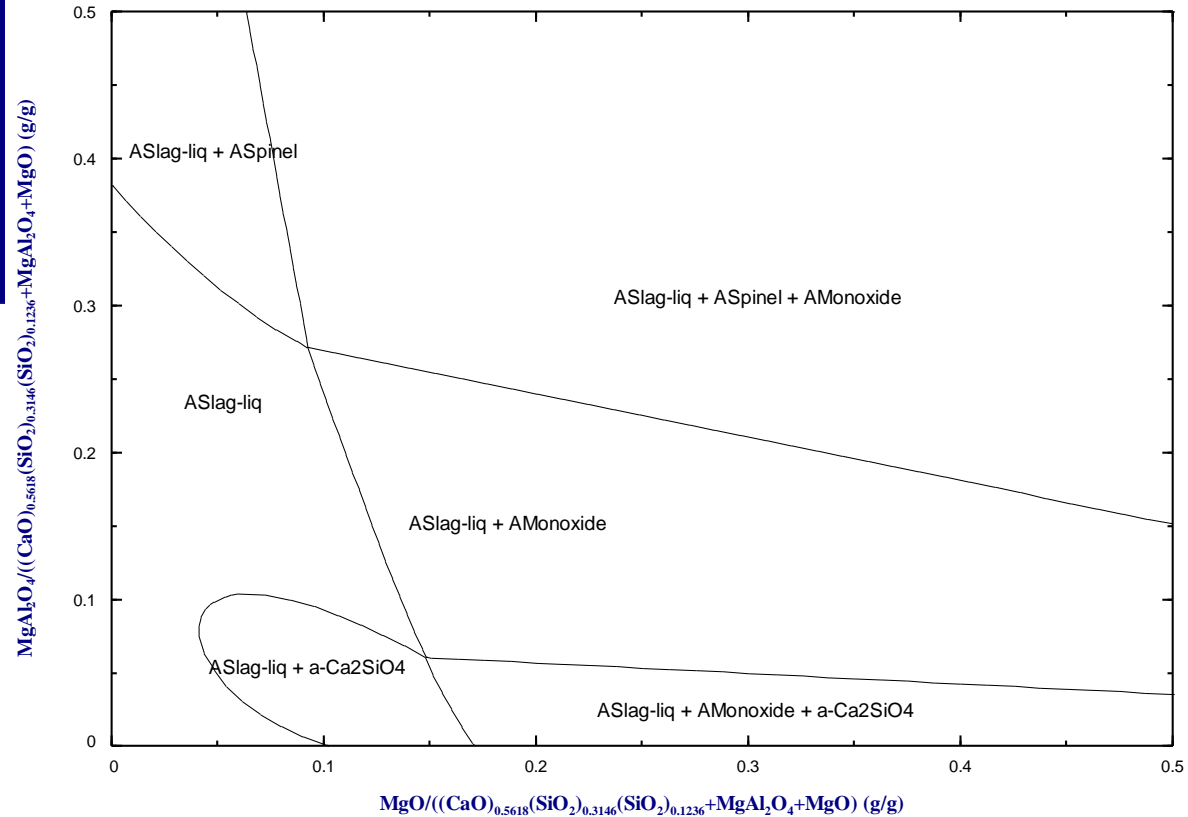
#1. L + M + MgO =

#1 log10(composition)

#2. L + M + MgO =

#2 log10(composition)

(CaO)_{0.5618}(SiO₂)_{0.3146}(SiO₂)_{0.1236} - MgAl₂O₄ - MgO
1600°C

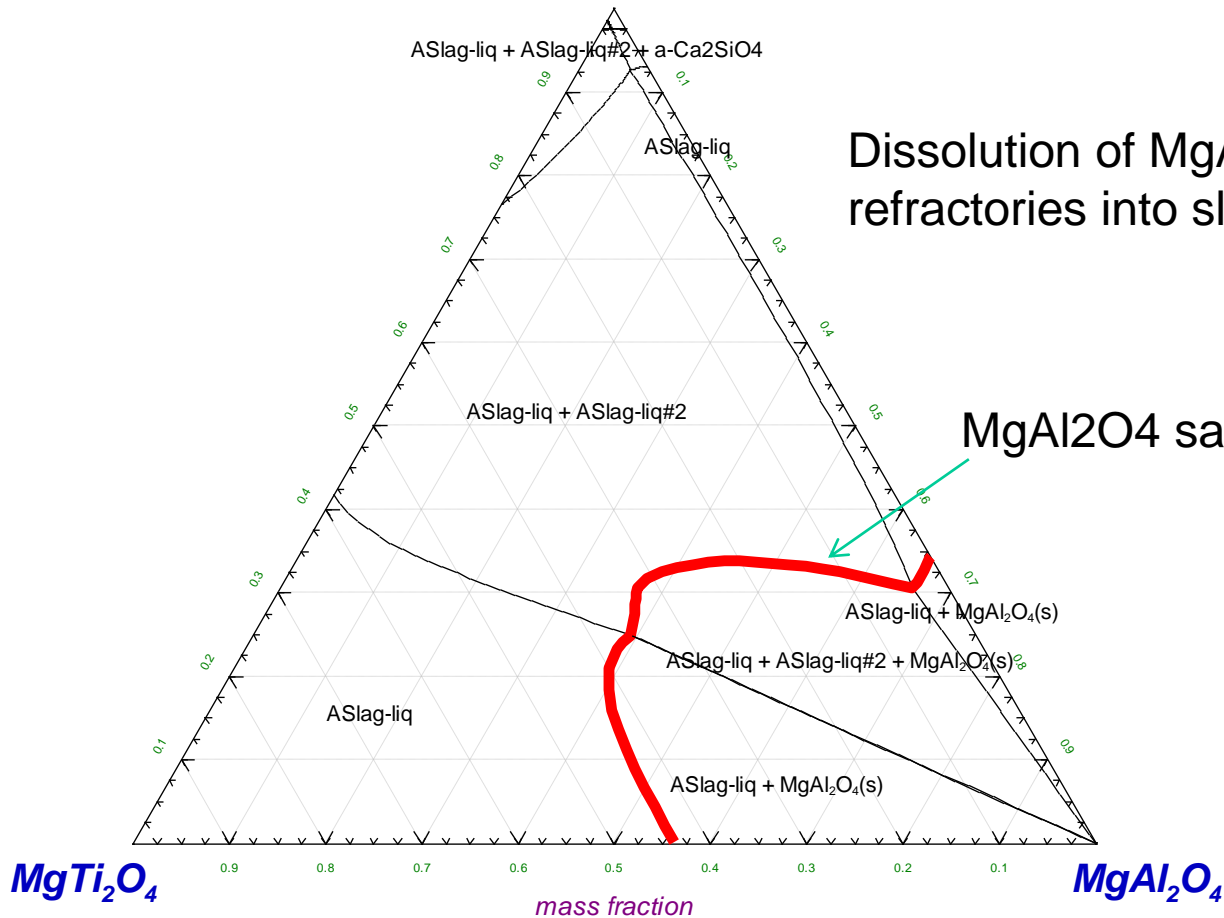


Phase diagram: Refractories design

$(\text{CaO})_{0.535}(\text{SiO}_2)_{0.25}(\text{Al}_2\text{O}_3)_{0.05}(\text{MgO})_{0.1} - \text{MgAl}_2\text{O}_4 - \text{MgTi}_2\text{O}_4 - \text{Fe}$
 1700°C, $a(\text{Fe}(\text{liq})) = 0.7943$



$(\text{CaO})_{0.535}(\text{SiO}_2)_{0.25}(\text{Al}_2\text{O}_3)_{0.05}(\text{MgO})_{0.1}$



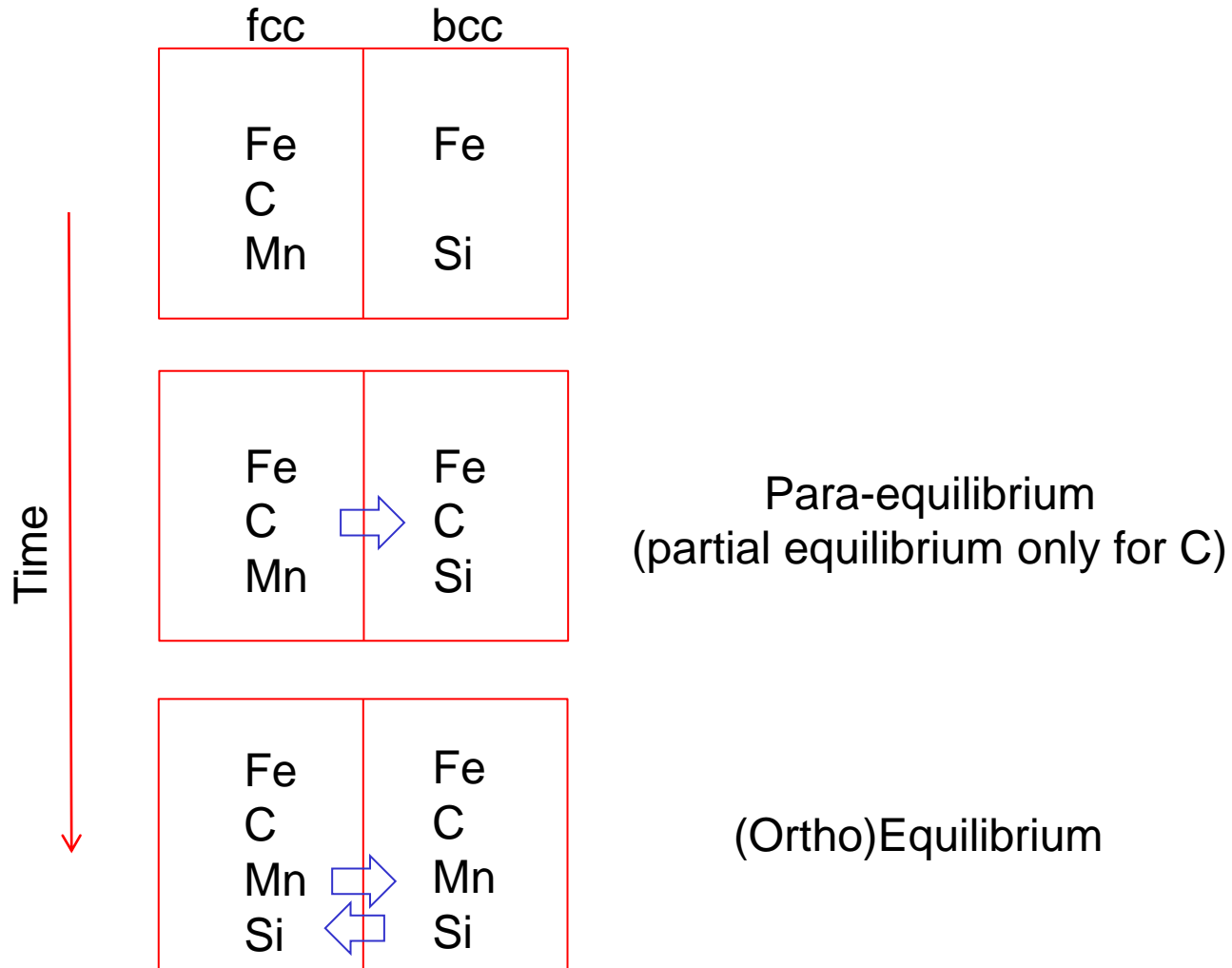
Dissolution of $\text{MgAl}_2\text{O}_4/\text{MgTi}_2\text{O}_4$ refractories into slag

MgAl₂O₄ saturation line

Para-equilibrium

Para-equilibrium (Partial equilibrium) vs Ortho-equilibrium (Fully equilibrium)

Diffusion of C is much faster than Mn or Si



Para-equilibrium: Steel A3 temperature

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

[gram] Fe + C + Mn

C is suppressed in the phase selection for convenience

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

* pure solids 14

* - custom selection species: 14

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FSstel-BCC	BCC_A2
	I	FSstel-HCP	HCP_A3
	+	FSstel-CEME	CEMENTITE
	+	FSstel-M23C6	M23C6
	+	FSstel-M7C3	M7C3
	+	FSstel-CBCC	CBCC_A12
	+	FSstel-CUB	CUB_A13
	+	FSstel-M5C2	M5C2

Legend

I - immiscible 4

+ - selected 6

Show all selected

species: 48

solutions: 14

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Virtual species: 6

Total Species (max 5000) 62

Total Solutions (max 200) 14

Total Phases (max 1500) 28

Variables

T(C)	C/(Fe+C+Mn)	Mn/(Fe+C+Mn)		
500 1000	0 0.02	0.02 (min)		

T(C) vs C/(Fe+C+Mn)

FactSage 8.0

Paraequilibrium diffusing elements

Y Enter the list of elements that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Mn C

C

OK

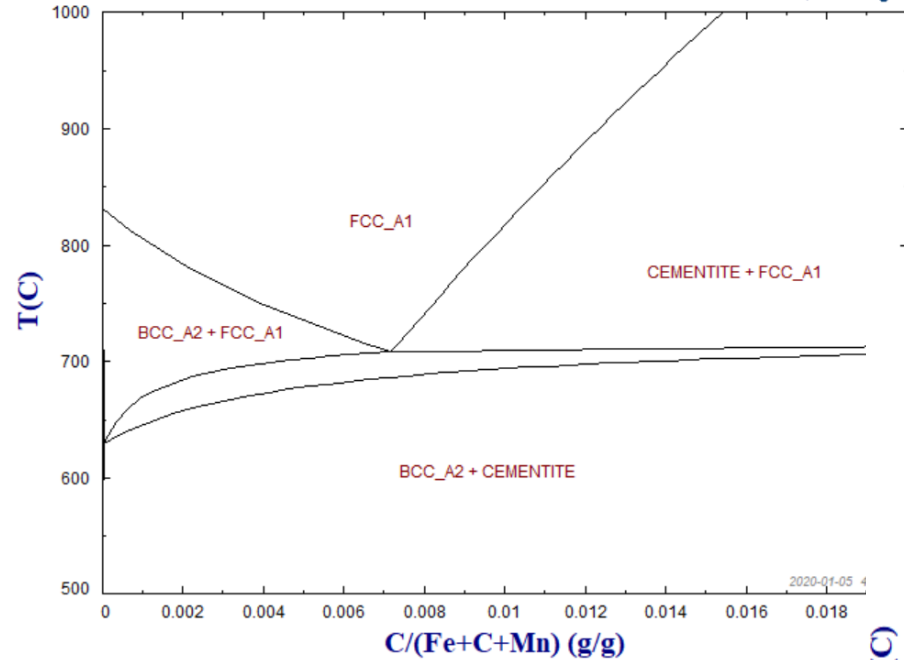
Cancel

Para-equilibrium: Steel A3 temperature

Full equilibrium

Fe - C - Mn

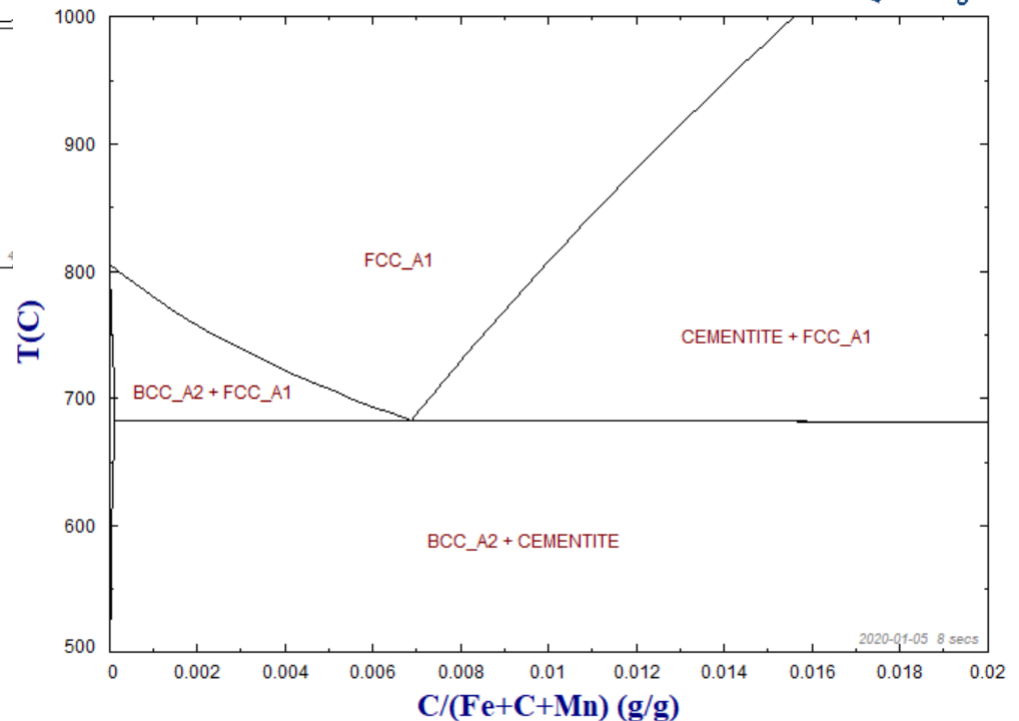
Mn/(Fe+C+Mn) (g/g) = 0.02, 1 atm



Para-equilibrium

Fe - C - Mn - paraequilibrium diffusing elements: C

Mn/(Fe+C+Mn) (g/g) = 0.02, 1 atm



Para-equilibrium: Rapid solidification for amorphous metal

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (2)

(gram) Cu + Zr

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 20

species: 20

Target

- none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-A1	FCC-A1
	I	FTlite-A2	BCC-A2
	I	FTlite-A3	HCP-A3
	I	FTlite-B2_a	BCC-B2a/BCC-A2
	I	FTlite-C11b	C11b Prototype-MoSi2
	I	FTlite-C15	C15 Prototype-MgCu2

Legend

I - immiscible 7

Show all selected

species: 36

solutions: 14

Paraequilibrium diffusing elements

Enter the list of elements that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Zr Cu

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 56

Total Solutions (max 200) 14

Total Phases (max 1500) 34

Phase Diagram

Y

X

- no time limit -

FactSage 8.0

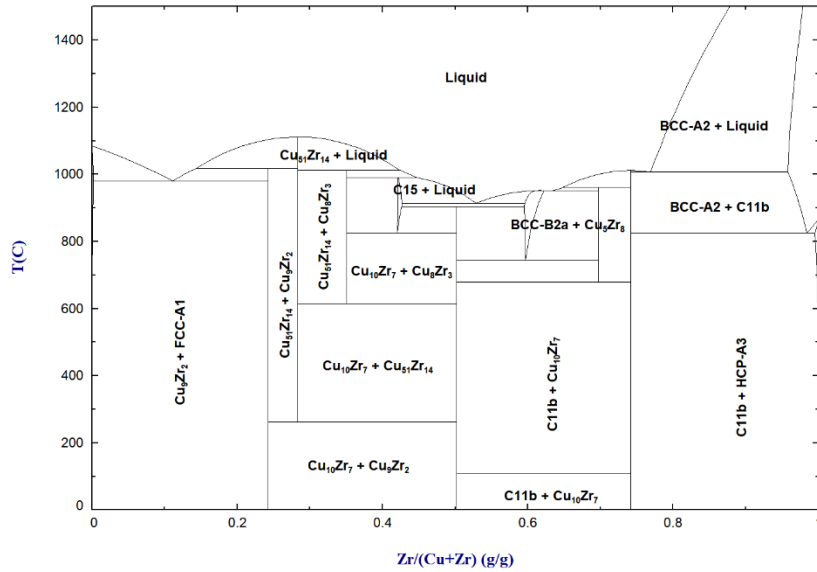
Blank → no diffusion of any element: this is what happens during rapid solidification

Para-equilibrium: Rapid solidification for amorphous metal

Full equilibrium

Cu - Zr
1 atm

FactSage™

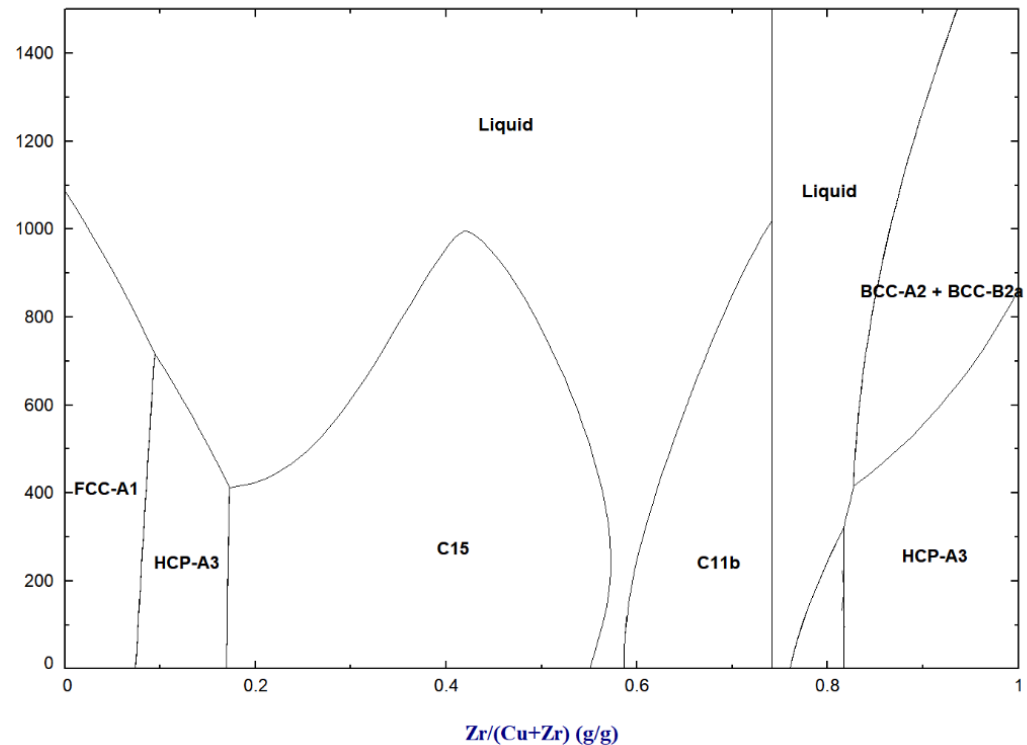


Paraequilibrium: Rapid solidification

Cu - Zr - phase with minimum G

1 atm

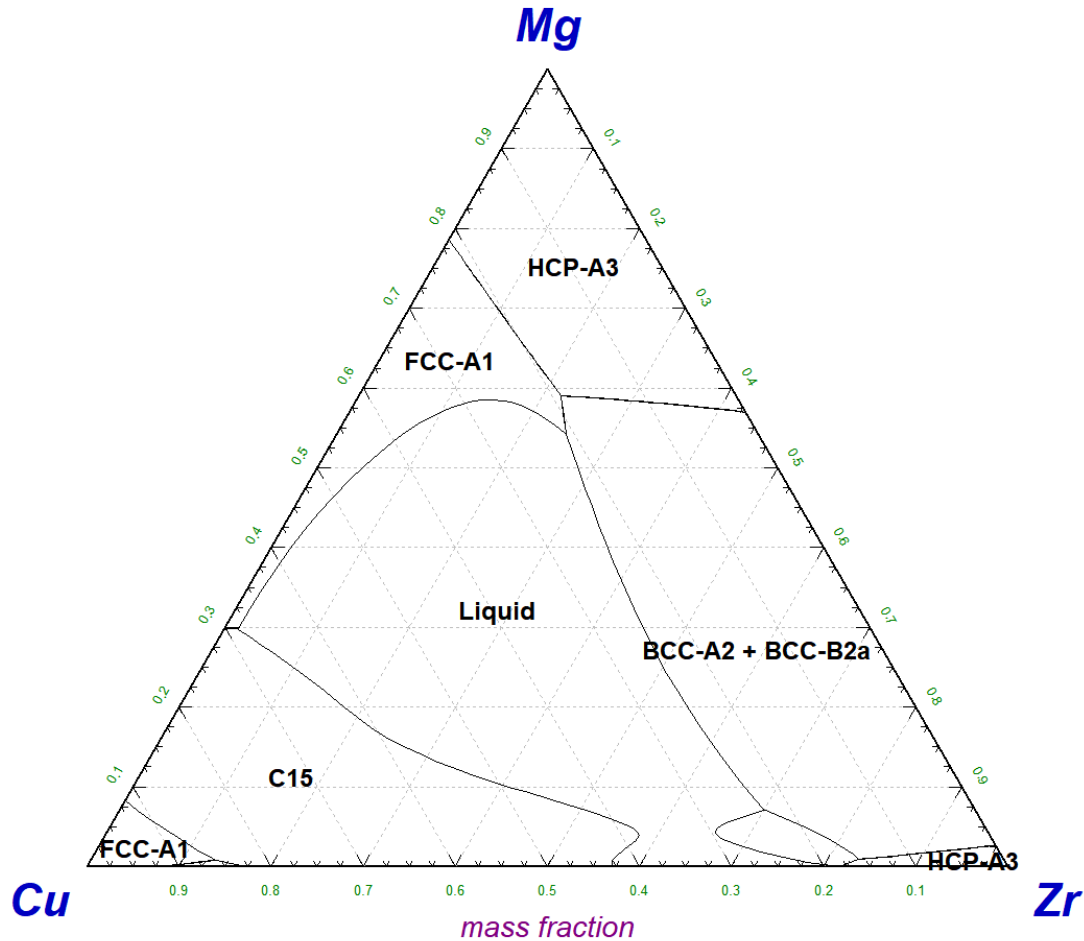
FactSage™



Para-equilibrium: Rapid solidification for amorphous metal

Mg - Zr - Cu - phase with minimum G

300°C, 1 atm

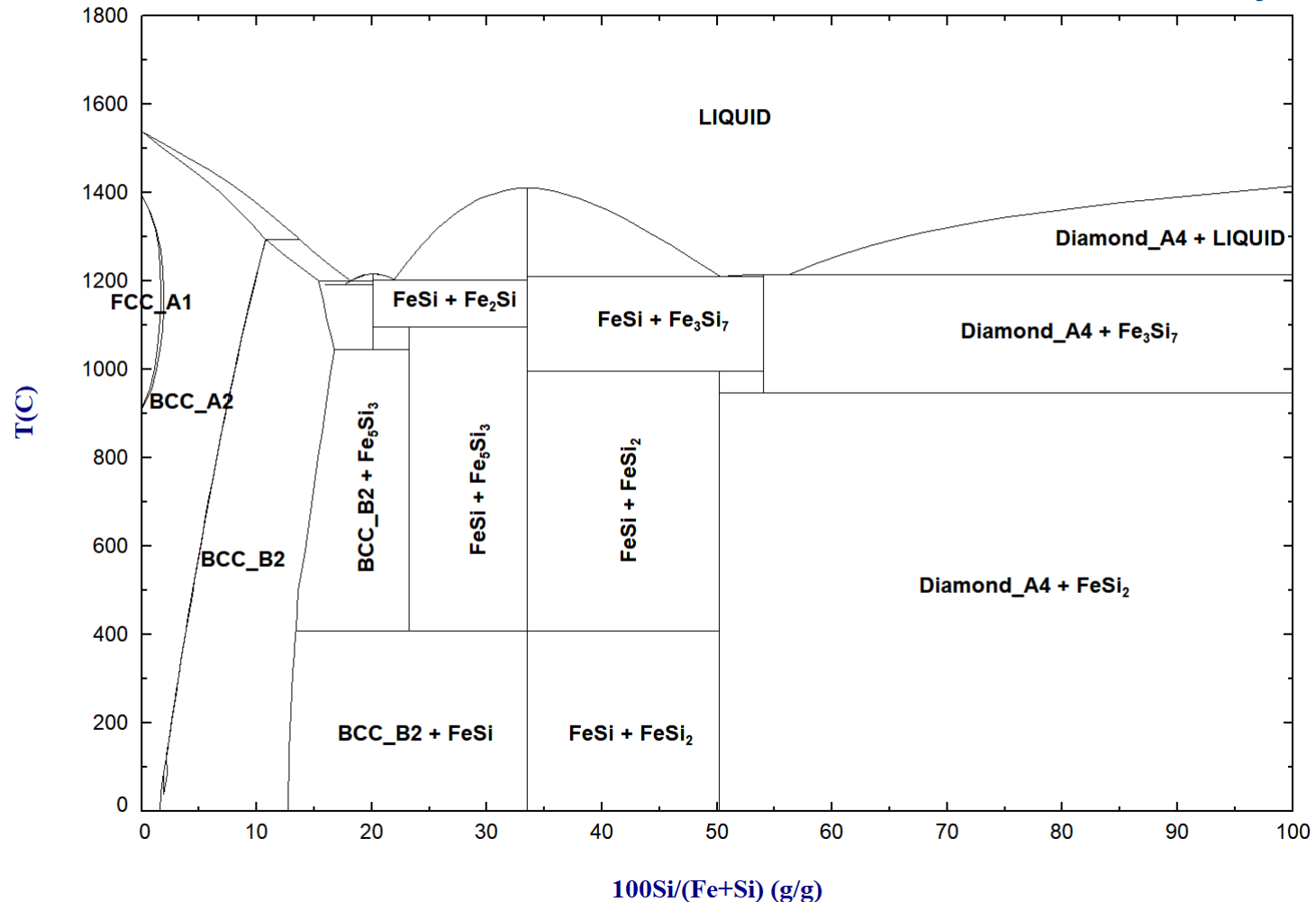


Alloy Design: Electric steel (Si-steel)

Phase diagram of Fe-Si system

Fe - Si

1 atm

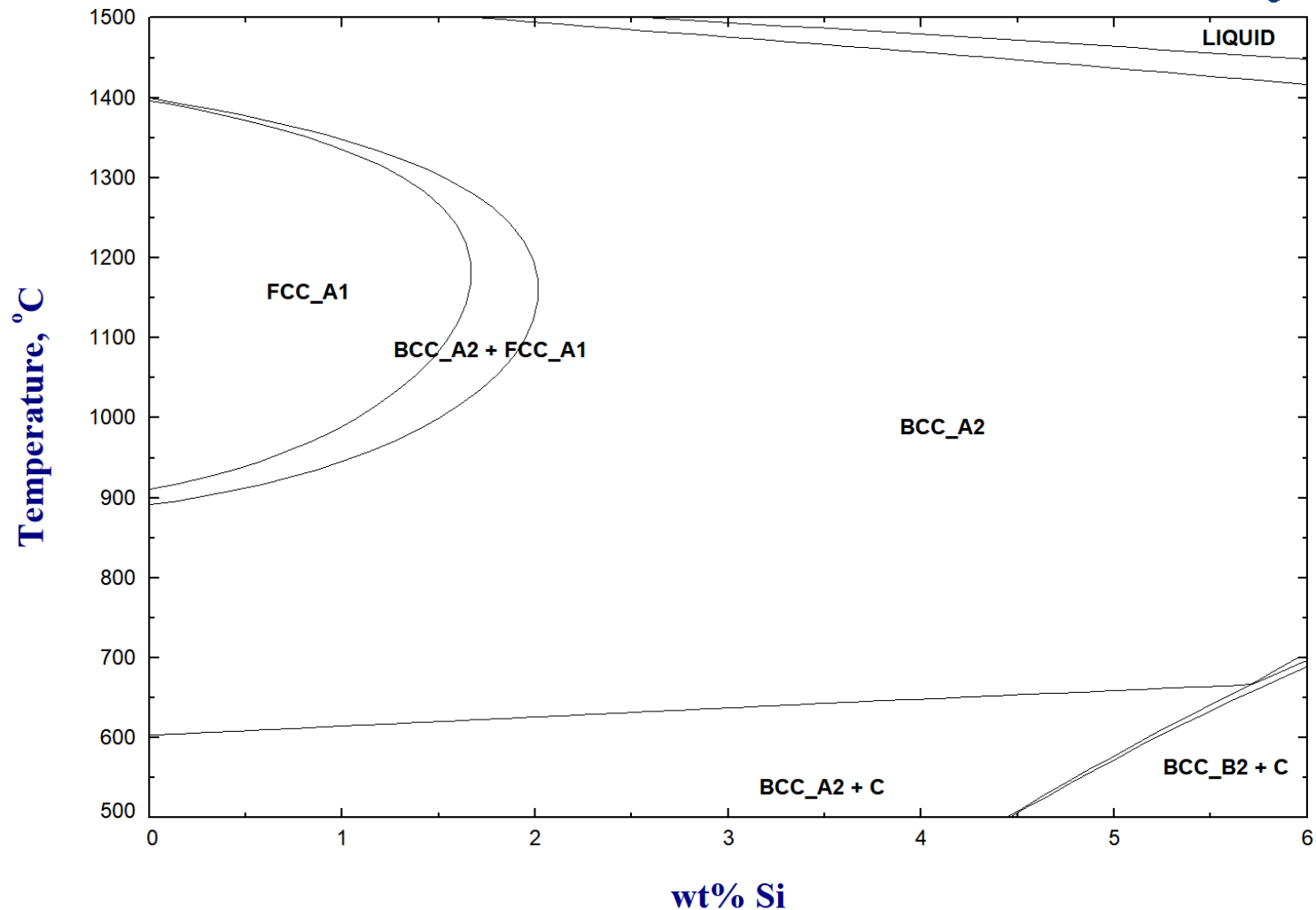


Alloy Design: Electric steel (Si-steel)

Alloy Design: Fe-Si + C

Fe - Si - C

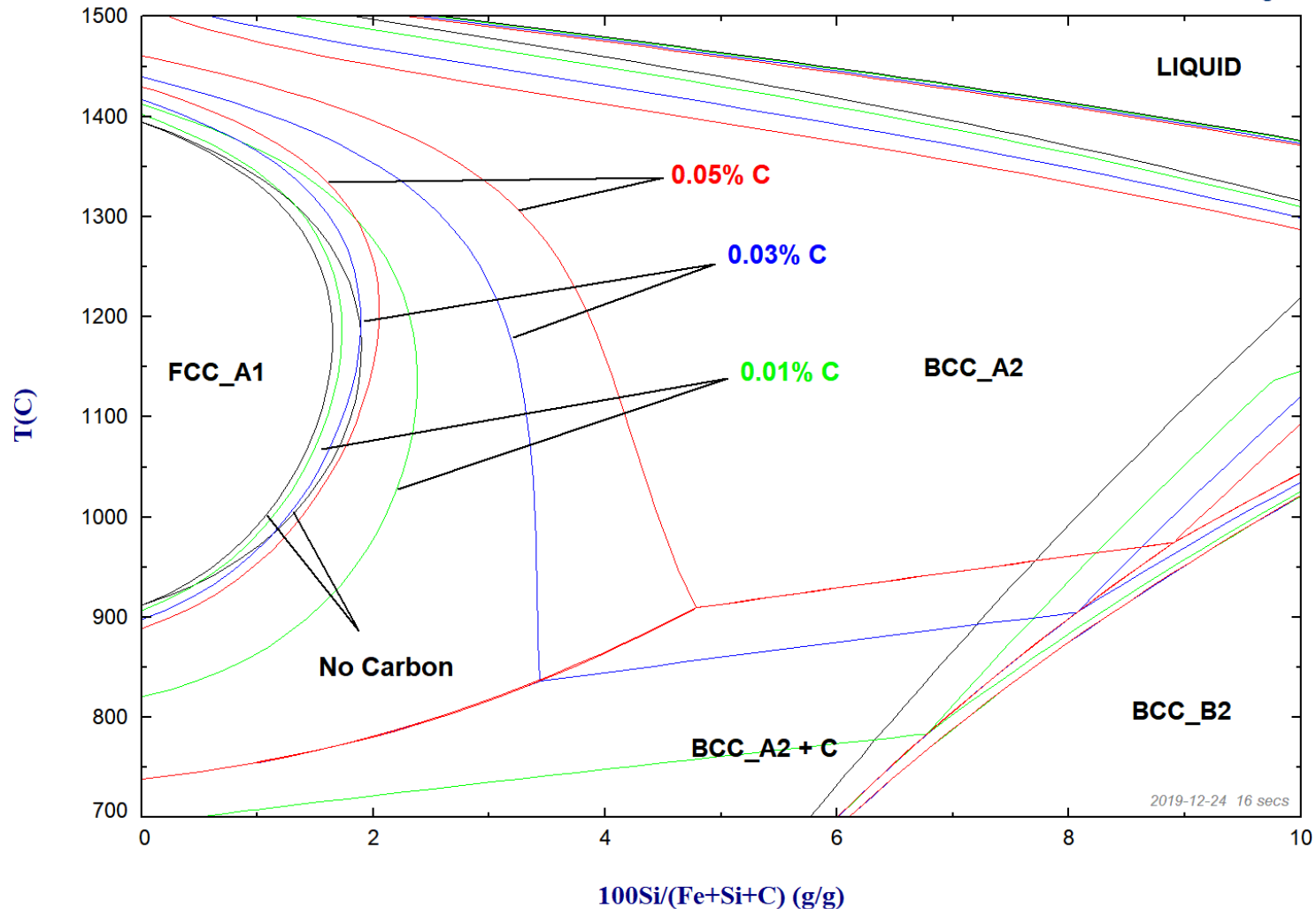
C = 25 ppm



Alloy Design: Electric steel (Si-steel)

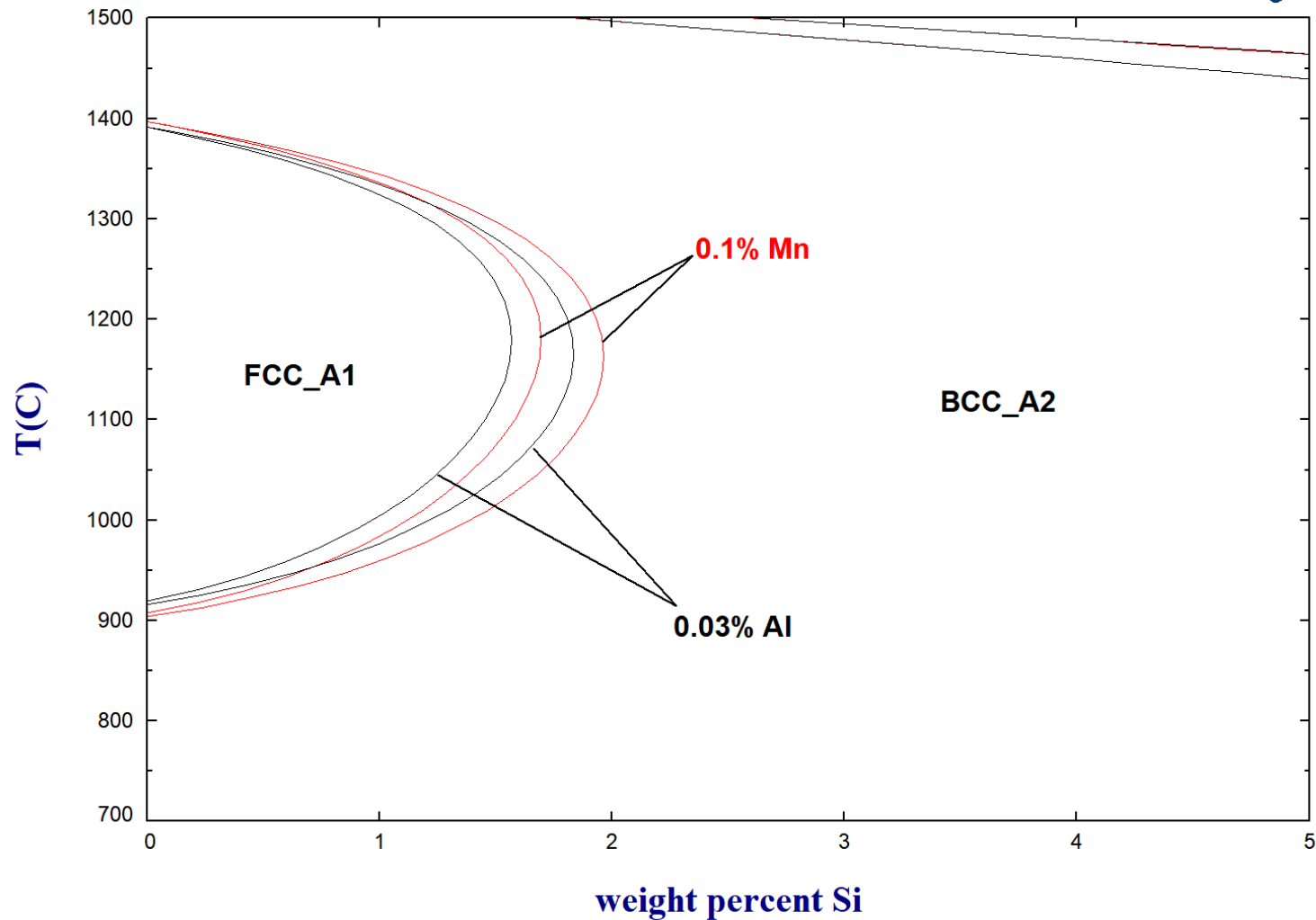
Alloy Design: Fe-Si + C

$100C/(Fe+Si+C) \text{ (g/g)} = 0, 1 \text{ atm}$

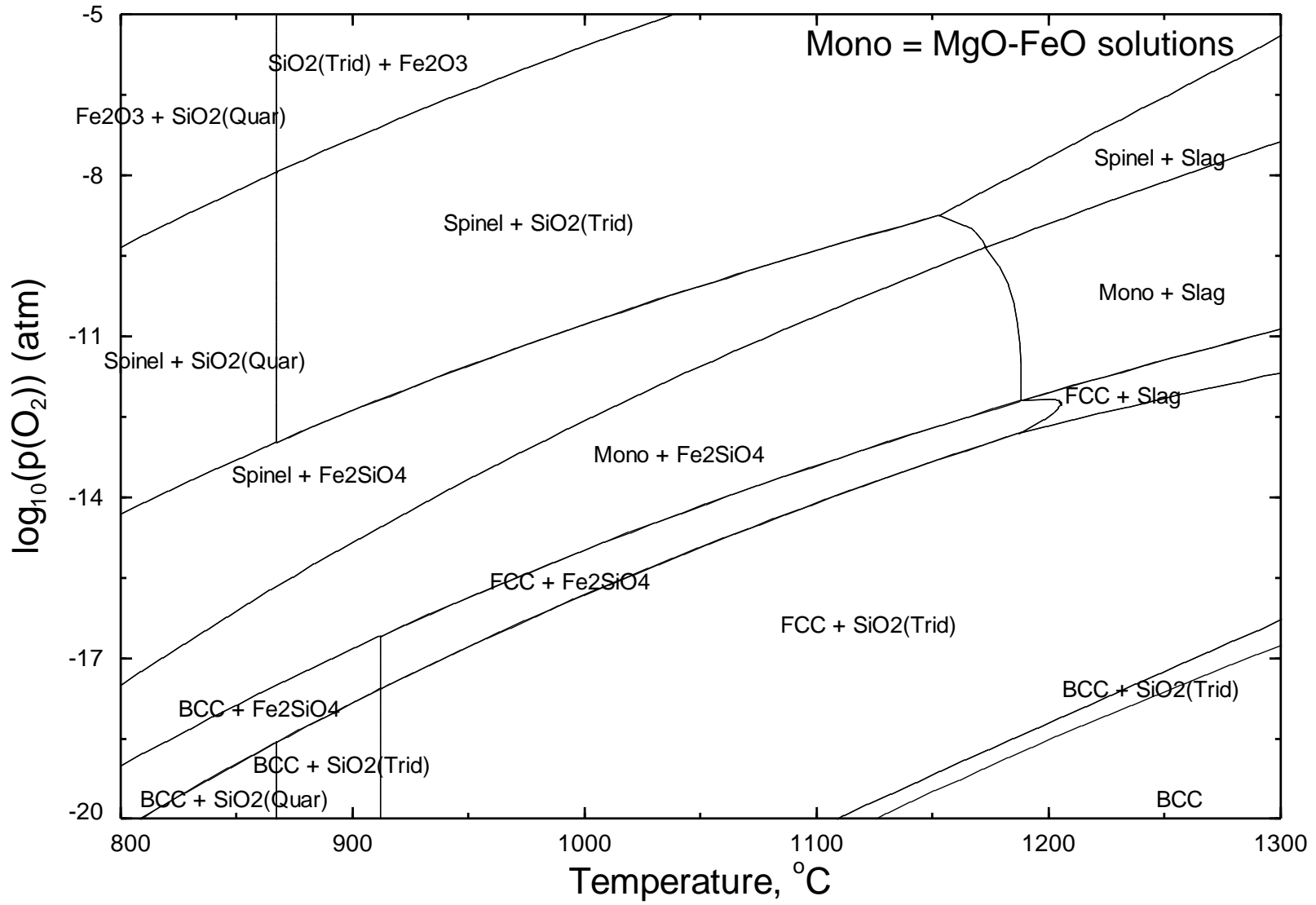


Alloy Design: Electric steel (Si-steel)

Alloy Design: Fe-Si + Al, Mn



Formation of base coating on the surface of a commercial Si steel



Thanks to FactSage Steelmaking Consortium Members

115



Visit In-Ho Jung's research group website
<http://in-ho-group.snu.ac.kr/>